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The 39th Annual Technical Meeting of the Society of Engineering Science (SES 2002) is scheduled to be held October 13-16, 2002 at the Nittany Lion Inn on the campus of Penn State University, State College, PA. The aim of the meeting is to provide a forum for exchanging ideas, methods, and results among researchers and educators in all fields of engineering science and mechanics. Over 340 invited and contributed abstracts have been accepted for presentation in 30 topical and special symposia In addition, plenary lectures and keynote presentations shall be given by distinguished scholars and representatives of several funding agencies. Topics included in the meeting include classical disciplines such as solid mechanics, fluid mechanics, dynamics, control, and materials processing/simulation as well as crosscutting areas of research such as quantum-continuum coupling and growth of biological tissues. Up to eight breakout sessions shall be run in parallel when plenary sessions are not underway.

This book provides an overview of the meeting, the titles and authors of all papers accepted for presentation, the body of all abstracts submitted by early-registered authors, an index of all authors of accepted papers, and a floor plan of the Nittany Lion Inn.

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SES 2002

The 39th Annual Technical Meeting of the Society of Engineering Science

Proceedings

October 13-16, 2002
State College, Pennsylvania

organized by

Department of Engineering Science & Mechanics
College of Engineering
The Pennsylvania State University

TABLE OF CONTENTS

Foreward

The 39th Annual Technical Meeting of the Society of Engineering Science (SES 2002) is scheduled to be held October 13-16, 2002 at the Nittany Lion Inn on the campus of Penn State University, State College, PA. The aim of the meeting is to provide a forum for exchanging ideas, methods, and results among researchers and educators in all fields of engineering science and mechanics. Over 340 invited and contributed abstracts have been accepted for presentation in 30 topical and special symposia. In addition, plenary lectures and keynote presentations shall be given by distinguished scholars and representatives of several funding agencies. Topics included in the meeting include classical disciplines such as solid mechanics, fluid mechanics, dynamics, control, and materials processing/simulation as well as cross-cutting areas of research such as quantum-continuum coupling and growth of biological tissues. Up to eight breakout sessions shall be run in parallel when plenary sessions are not underway.

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The organizers of the meeting gratefully acknowledge the financial support of several entities: the Department of Engineering Science and Mechanics at Penn State for underwriting certain costs of the meeting, the US Office of Naval Research and the College of Engineering at Penn State for support of the Student Paper Competition, and the US Air Force Office of Scientific Research for support of the Student Design-Build Challenge. The SES officers and members of the Board of Directors are thanked for their encouragement and advice. The hard work of the Program Committee in organizing symposia and reviewing abstracts is greatly appreciated. The session chairs are thanked for ensuring the smooth running of their sessions. The behind-the-scenes work done by the meeting support staff, especially Mr. Terry Reed and Mr. Andrew Arvin, is gratefully acknowledged. Above all, the participants are thanked for contributing to the success of the meeting.

C.E. Bakis, Technical Program Chair (email: cbakis@psu.edu)
3 October 2002

Department of Engineering Science & Mechanics
212 Earth-Engineering Science Bldg.
Penn State University
University Park, PA 16802-6812
Tel. (814) 865-4523

Awards and Honors

William Prager Medal — Prof. S. Nemat-Nasser, University of California - San Diego

Student Paper Competition

The Student Paper Competition is being sponsored by the US Office of Naval Research and the Penn State College of Engineering. The support of this event by Dr. Yapa D. S. Rajapakse, Program Manager of the Ship Structures Division, and Dr. David N. Wormley, Dean of the College of Engineering, is greatly appreciated. Ten presentations were selected based on abstracts submitted by 20 applicants. The schedule for the Student Paper Competition is given on page 8.

Conference Organization

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Technical Program

Format of Program

The technical program begins with an overview of meeting events on page 6. Plenary and Keynote sessions are listed first, followed by special symposia, the Student Paper Competition, and the topical symposia by number. Next is a detailed list of concurrent sessions organized by session name. Paper titles and authors are included in the list of concurrent sessions. Abstracts of early-registered authors appear next, organized by symposium. The abstracts have page numbers such as "X-Y," where "X" is the symposium number and "Y" is the page number within symposium "X." The abstracts are ordered in accordance with the schedule in effect at the time this book was printed. Some changes to the final schedule are inevitable. Persons interested in attending particular presentations should check the most up-to-date schedule posted outside each breakout room and near the meeting registration desk.

Session Name Code

Sessions are named by a code consisting of two letters and a number, as follows:

1st letter refers to the day of the session
- M: Monday, October 14
- T: Tuesday, October 15
- W: Wednesday, October 16

2nd letter refers to time of the session
- A: Morning session
- B: 1st afternoon session
- C: 2nd afternoon session

Session MA2

The number refers to the location of the session
1: Boardroom-1
2: Fireside Lounge
3: Ballroom-A
4: Ballroom-B
5: Boardroom-2
6: Ballroom-D
7: Ballroom-E
8: Mt. Nittany Room

Overview of Meeting

All event locations are in the Nittany Lion Inn unless otherwise designated.

Sunday, October 13, 2002

9:00 – 12:00	SES Awards Committee Meeting, Penn State Room
1:00 – 5:00	SES Board of Directors Meeting, Penn State Room
4:30 – 7:30	Registration, Rotunda Lobby
6:30 – 8:00	Reception, Alumni Lounge/Lobby

Monday, October 14, 2002

7:00 – 5:00	Registration, Rotunda Lobby
7:45 – 8:00	Welcome, Ballroom C
8:00 – 8:55	Prager Medalist Lecture: Prof. Siavouche Nemat-Nasser *Multifunctional Materials/Structures: A New Horizon in Engineering Science* Location: Ballroom C
9:00 – 5:00	Design-Build Challenge, 312/314 Hammond Bldg.
8:55 – 9:15	Break
9:15 – 11:20	Technical Sessions MA1 – MA8
11:20 – 12:35	Lunch (on own)
12:35 – 2:40	Technical Sessions MB1 – MB8
2:40 – 2:55	Break
2:55 – 5:50	Technical Sessions MC1 – MC8

Tuesday, October 15, 2002

7:00 – 5:00	Registration, Rotunda Lobby
8:00 – 8:55	Plenary Lecture: Prof. Ted Belytschko *Meshless and Extended Finite Element Methods in Mechanics* Location: Ballroom C
9:00 – 5:00	Design-Build Challenge, 312/314 Hammond Bldg. Final Competition 4:00-5:00 in lobby of Earth-Engineering Sciences Bldg.
8:55 – 9:15	Break
9:15 – 11:20	Technical Sessions TA1 – TA8
11:20 – 12:35	Lunch (on own)
12:35 – 2:40	Technical Sessions TB1 – TB8
2:40 – 2:55	Break
2:55 – 5:00	Technical Sessions TC1 – TC8
6:30 – 7:00	Reception, Atrium
7:00 – 9:30	Banquet, Ballroom

Wednesday, October 16, 2002

7:00 – 1:00	Registration, Rotunda Lobby
8:00 – 8:55	Plenary Lecture: Prof. Kumbakonam R. Rajagopal *On the Mechanics of Growth and Adaptation in Biological Materials* Location: Ballroom C
8:55 – 9:15	Break
9:15 – 11:20	Technical Sessions WA1 – WA6
11:20 – 12:35	Lunch (on own)
12:35 – 2:40	Technical Sessions WB1 – WB6
2:40 – 2:55	Break
2:55 – 5:00	Technical Sessions WC1 – WC8

Plenary Lectures

Monday, October 14, 8:00-8:55 AM, Location: Ballroom C (Chair: R.P. McNitt)

Prof. Siavouche Nemat-Nasser, University of California - San Diego
(SES 2002 William Prager Medalist)

Multifunctional Materials/Structures: A New Horizon in Engineering Science

Tuesday, October 15, 8:00-8:55 AM, Location: Ballroom C (Chair: N.J. Salamon)

Prof. Ted Belytschko, Northwestern University

Meshless and Extended Finite Element Methods in Mechanics

Wednesday, October 16, 8:00-8:55 AM, Location: Ballroom C (Chair: C.E. Bakis)

Prof. Kumbakonam R. Rajagopal, Texas A&M University

On the Mechanics of Growth and Adaptation in Biological Materials

Keynote Presentations

Monday, October 14, 10:30-11:20 AM, Location: Assembly Room (Chair: T.J. Mackin)

Prof. Jacob Israelachvili, University of California – Santa Barbara

Equilibrium Versus Non-Equilibrium Assembly of Nano-Structures in Solution

Monday, October 14, 2:55-3:45 PM, Location: Assembly Room (Chair: W.A. Curtin)

Dr. Yapa D. S. Rajapakse, Program Manager, Ship Structures Division, U.S. Office of Naval Research

Challenges and Recent Advances in Composites for Marine Structures

Tuesday, October 15, 10:30-11:20 AM, Location: Assembly Room (Chair: G.A. Lesieutre)

Dr. Gary Anderson, Structural Mechanics Branch, Mechanical and Environmental Sciences Division, U.S. Army Research Office

ARO Programs in Mechanical and Environmental Sciences

Tuesday, October 15, 2:55-3:45 PM, Location: Assembly Room (Chair: N.J. Salamon)

Dr. Vasundara Varadan, Division Director, Electrical and Communications Systems, U.S. National Science Foundation

Challenges and Opportunities in Engineering Research and Education—an NSF Perspective

Wednesday, October 16, 10:30-11:20 AM, Location: Assembly Room (Chair: C.E. Bakis)

Dr. B. "Les" Lee, Program Manager, Mechanics of Materials and Devices, U.S. Air Force Office of Scientific Research

AFOSR Research Programs in the Area of Mechanics of Materials and Devices

Special Symposia

Special Symposium in Honor of SES 2002 Prager Medalist

S. Nemat-Nasser Symposium (Symposium No. 15)
Organizers: John R. Willis, Cambridge University
Mohammed Zikry, North Carolina State University
Sessions: MA1, MB1, MC1, TA1
Location: Boardroom-1

Special Symposium in Honor of Professor A. Cemal Eringen on the Occasion of His 81st Birthday

A.C. Eringen Symposium (Symposium No. 7)
Organizers: Mysore N.L. Narasimhan
A.D. Kirwan, Jr., University of Delaware
Sessions: MA2, MB2, MC2, TA2, TB2, TC2
Location: Fireside Lounge

Student Paper Competition

Sponsored by the US Office of Naval Research and the Penn State College of Engineering

Symposium No.: 18
Organizers: William Thompson, Jr., and Charles E. Bakis, Penn State University
Sessions (Location): TA3, TB3 (Ballroom-A). Awards given at banquet.

Finite Strain Response and Texture Evolution of α- and β-Crystalline Polypropylene, W. Xu, E.M. Arruda – Univ. of Michigan (USA)

Thermodynamic Framework for Coupling of Non-Local Viscoplasticity and Non-Local Anisotropic Viscodamage for Dynamic Localization Problems Using Gradient Theory, R.K. Abu Al-Rub, G.Z. Voyiadjis, A.N. Palazotto – Louisiana State Univ. (USA)

Strain Rate Sensitivity of Cymat Aluminum Foam Subject to Uniaxial Compressive Loading, M.M. Braun, K.A. Issen – Clarkson Univ. (USA)

Experimental Analysis of Compaction Band Formation in Aluminum Foam Using Surface Strain Mapping, T.P. Casey, K.A. Issen – Clarkson Univ. (USA)

Tissue Engineering and Characterization of Self-Organized Tendon Constructs, S. Calve, R.G. Dennis, K. Grosh, E.M. Arruda – Univ. of Michigan (USA)

Conditions for Localized Compaction in High Porosity Sandstone, V. Challa – Clarkson Univ. (USA)

Low K Dielectric Thin Film Development and High Frequency Characterization, H.-P. Hsueh, M.T. Lanagan, R.T. McGrath – Penn State Univ. (USA)

Tool Condition Monitoring, S. Jayasankar – Osamnia Univ. (India)

Nanoindentation of Alumina Matrix – Chrome Carbide Nanoparticles Composite, L. Yerakhavets, M. Kireitseu, I. Nemerenco – Institute of Machine Reliability (Belarus)

Rheological Behavior and Model of Alumina-Polymer-Based Composites, I. Nemerenco, M. Kireitseu, L. Yerakhavets – Institute of Machine Reliability (Belarus)

Student Design/Build Challenge

Sponsored by the US Air Force Office of Scientific Research

Teams of university undergraduate and high school students will apply principles of engineering science to design and build remote-controlled lighter-than-air vehicles to traverse an above-ground course. Support of this event by Dr. B. "Les" Lee, Program Manager of Mechanics of Materials and Devices, AFOSR, is greatly appreciated. The schedule follows.

Date/Time	Activity	Location
Monday 9:00-4:00	Design and Build	312/314 Hammond Bldg.
Monday 4:00-5:00	ESM Dept. Laboratory Tours	Leave from 312/314 Hammond Bldg.
Tuesday 9:00-10:00	ESM Dept. Laboratory Tours	Leave from 312/314 Hammond Bldg.
Tuesday 10:00-3:00	Design and Build	312/314 Hammond Bldg.
Tuesday 3:00-5:00	Test and Compete	Lobby of Earth-Engineering Sciences Bldg. (competition to start at 4:00)

Topical Symposia by Number

Following is information for each topical symposium: title, number, session name, room, and organizers. The symposia are listed in ascending numerical order. A list of individual papers accepted for presentation is given under "Concurrent Sessions" beginning on page 11.

Symposium Title (number)	Session Name (Room)	Organizers
Active and Passive Models of Biological Tissue & Functional Engineered Tissue (1)	MA8, MB8 (Mt. Nittany Room)	Ellen M. Arruda and Karl Grosh, Univ. of Michigan
Compliant Mechanisms (2)	MA7 (Ballroom-E)	Mary I. Frecker, Penn State Univ., and G.K. Ananthasuresh, Univ. of Pennsylvania
Continuum Plasticity and Damage Mechanics (3)	WA3, WB3, WC3 (Ballroom-A)	Cliff J. Lissenden, Penn State Univ., and George Z. Voyiadjis, Louisiana State Univ.
Discrete to Continuum: Mechanical Modeling Across Scales (4)	MA3 (Ballroom-A)	Gary L. Gray and Francesco Costanzo, Penn State Univ.
Dynamic Fracture (5)	MB3, MC3 (Ballroom-A)	Francesco Costanzo, Penn State Univ., and Jay R. Walton, Texas A&M Univ.
Dynamical Systems Methods for Advanced Diagnostics and Prognostics (6)	MA5, MB5, MC5 (Boardroom-2)	Joseph P. Cusumano, Penn State Univ., and David Chelidze, Univ. of Rhode Island
Fractional Derivatives in Viscoelasticity (8)	WB1, WC1 (Boardroom-1)	George A. Lesieutre, Penn State Univ. and Mikael Enelund, Chalmers Univ. Tech.
Growth in Biological Tissues (9)	TB8 (Mt. Nittany Room)	I. Joga Rao, New Jersey Inst. of Tech., and Grama Praveen, General Electric Corporate R&D
Mechanics and Physics of Solid-Solid Phase (10)	MB6, MC6 (Ballroom-D)	Dimitris C. Lagoudas, Texas A&M Univ., Valery I. Levitas, Texas Tech Univ., and Ibrahim Karaman, Texas A&M Univ.

Topical Symposia by Number (cont.)

Micro- and Nano-Scale Engineering (11)	MA4, MB4 (Ballroom-B)	Thomas J. Mackin, Univ. of Illinois – Urbana-Champaign
Nanoscale Science and Technology (12)	MC4 (Ballroom-B)	Akhlesh Lakhtakia, Penn State Univ.
Particle Systems (13)	TB1, TC1, WA1 (Boardroom-1)	Virendra M. Puri, Penn State Univ., and J. Guadalupe Arguello, Sandia Natl. Laboratories
Polymer Mechanics (14)	WA8, WB8 (Mt. Nittany Room)	I. Joga Rao, New Jersey Inst. of Tech., and Grama Praveen, General Electric Corporate R&D
Quantum/Atomistic/Continuum Coupling in Materials Simulation (16)	TA5, TB5, TC5, WA5, WB5 (Boardroom-2)	Harley Johnson, Univ. of Illinois – Urbana-Champaign, and William A. Curtin, Brown Univ.
Simulation Based Control (17)	TC3 (Ballroom-A)	Richard A. Wysk, Penn State Univ. and Young-Jun Son, Univ. of Arizona
Synergistic Enviro-Mechanical Degradation Kinetics and Acceleration (19)	TA8 (Mt. Nittany Room)	John J. Lesko, Virginia Tech, and Andras Szekeres, TU Budapest
Thermo-Mechanical Problems (20)	TA7, TB7 (Ballroom-E)	Panagiotis Michaleris, Penn State Univ., and Nicholas Zabaras, Cornell University
Ultrasonic NDE (21)	WA2, WB2, WC2 (Fireside Lounge)	Joseph L. Rose and Chiaki Miyasaka, Penn State Univ.
Wear and Tribology (22)	TA4, TB4, TC4, WA4 (Ballroom-B)	Albert E. Segall, and Joseph Conway, Penn State Univ.
X-ray Computed Tomography in Materials Science & Engineering (23)	WA6, WB6, WC6 (Ballroom-D)	Nevin L. Rupert and Joseph M. Wells, US Army Research Laboratory
General Topics (24)	MA6 (Ballroom-D), TC7 (Ballroom-E), WC5 (Boardroom-2)	Charles E. Bakis, Penn State Univ.
Multiscale Modeling of Solidification (25)	WA7, WB7, WC7 (Ballroom-E)	Mark F. Horstemeyer, Sandia Natl. Laboratories, and Douglas B. Kothe, Los Alamos Natl. Laboratory
Recent Advances in Ceramic Matrix Composites for Aeronautics & Aerospace (26)	WB4 – Closed*, WC4 – Open (Ballroom-B)	Roy M. Sullivan, NASA Glenn Research Center
*Session WB4 is closed to all persons except those who fill out an ITAR Restricted Data Nondisclosure Agreement form and present the form and any necessary documentation at the session. Note that permanent resident aliens must present their green card in order to gain access to the closed session. The form is available at the registration desk and at the meeting website under the page with information for this symposium: http://www.esm.psu.edu/ses2002/symposia/37.html		
Materials Modeling Issues for Engineering Systems (27)	TC8 (Mt. Nittany Room)	David Lo and Bill Scherzinger, Sandia Natl. Laboratories
Structural Dynamics and Stability (28)	TA6, TB6, TC6 (Ballroom-D)	Eric Mockensturm, Penn State Univ., and Arvind Raman, Purdue Univ.
Thermomechanics of the Inelastic Behavior of Materials (29)	MB7, MC7 (Ballroom-E)	Arun Srinivasa and K. R. Rajagopal, Texas A&M Univ.
Cell and Molecular Bioengineering (30)	MC8 (Ballroom-E)	Peter Butler and Cheng Dong, Penn State Univ.

Concurrent Sessions

All accepted papers are listed below according to the schedule in effect when this book was printed. Some changes to the final schedule are inevitable. Persons interested in attending particular presentations should check the most up-to-date schedule posted outside each breakout room and near the meeting registration desk.

Concurrent Sessions — Monday A, 9:15–11:20 AM

MA1 Boardrm-1	*S. Nemat-Nasser Symposium (15)*	Organizers: J.R. Willis, M. Zikry Chairs: J.R. Willis, M. Zikry
9:15-9:40	*Stress Amplification in Thin Ligaments*, X. Markenscoff	
9:40-10:05	*Second-Order Homogenization Estimates for Viscoplastic Polycrystals*, P. Ponte Castaneda, Y. Liu	
10:05-10:30	*Heat Transfer Properties of Graphite Foam*, N. Yu, C.C. Tee, H. Li	
10:30-10:55	*Boundary-Layer Corrections for Stress and Strain Fields in Randomly Heterogeneous Media*, R. Luciano, J.R. Willis	
10:55-11:20	*Micromechanics of Ferroelectric Polymer Based Electrostrictive Composites*, J. Li, N. Rao	

MA2 Fireside	*A.C. Eringen Symposium (7)*	Organizers: M.N.L. Narasimhan, A.D. Kirwan, Jr. Chair: A. D. Kirwan, Jr.
9:15-9:40	*A Mathematical Model of Pulsatile Flows of Microstretch Fluids in Circular Tubes,* M.N.L. Narasimhan	
9:40-10:05	*Asymptotic Behavior of Micropolar Fluid Flows,* G. Lukaszewicz	
10:05-10:30	*Probabilistic Design Analysis of Fluid Structure Interaction,* R.S.R. Gorla, S.S. Pai	
10:30-10:55	*Advances in Crystal Growth from the Liquid Phase,* S. Dost	
10:55-11:20	*Model Reduction of Large Space Structures Using Approximate Component Cost Analysis,* K. Grigoriadis, I. Kunin	

MA3 Ballrm-A	*Discrete to Continuum: Mechanical Modeling Across Scales (4)*	Organizers: G.L. Gray, F. Costanzo Chairs: G.L. Gray, F. Costanzo
9:15-9:40	*An Atomistic Model-Based Continuum Analysis Incorporating the Finite Temperature Effect,* Y. Huang, H. Jiang	
9:40-10:05	*Deriving Continuum Properties from MD Simulations for Columnar Thin Films,* G.L. Gray, F. Costanzo, T.J. Yurick Jr., P. Andia	
10:05-10:30	*A Multiscale Continuum Mechanics Model for Predicting Damage Evolution in Inelastic Heterogeneous Media,* D.H. Allen	
10:30-10:55	*Connecting Discrete Atomic Model to Microcontinuum Field Theories,* Y. Chen, J.D. Lee, A. Eskandarian	
10:55-11:20	*Rheology and Fluid Dynamics of Micellar Solutions,* L. Berlyand, E. Khrsulov	
11:20-11:45	*Homogenization of Polymer-Based Nanocomposites,* R.C. Picu, A. Sarvestani, M.S. Ozmusul	

MA4 Ballrm-B	*Nanoscale Science and Technology (12)*	Organizer: A. Lakhtakia Chair: A. Lakhtakia
9:15-9:40	*Sphere Packings, Order Metrics, and Jamming,* S. Torquato	
9:40-10:05	*Controlled Column Tilt Angle Using Non-uniform Substrate Rotational Speed in Glancing Angle Deposition,* D. Ye, Y. Zhao, G. Yang, G.-C. Wang, T.-M. Lu	
10:05-10:30	*Nominal Microstructure--Based Model for Chiral Sculptured Thin Films: Dielectric and Bianisotropic Properties,* J.A. Sherwin, A. Lakhtakia	
10:30-10:55	*Retardation of Oxidation in Co Nano-Columns,* J.P.Singh, F. Tang, D.-X. Ye, T.-M. Lu, G.-C. Wang	
10:55-11:20	*Investigation of the Stress Corrosion Cracking, Corrosion Fatigue and Localized Corrosion Resistance of Conventional and Nanostructured Al-Mg Alloys,* M.M. Sharma-Judd, B.A. Shaw, E. Sikora	
11:20-11:45	*Rheological Behavior and Fatigue of Alumina-Chrome Carbide Nanoparticles Nanostructures and Nanocomposites,* M. Kireitseu, L. Yerakhavets, I. Nemerenco	

(more Monday A on next page)

Concurrent Sessions — Monday A, 9:15–11:20 AM

MA5 Boardrm-2	*Dynamical Systems Methods for Advanced Diagnostics and Prognostics (6)*	Organizers: J.P. Cusumano, D. Chelidze Chairs: J.P. Cusumano, D. Chelidze
9:15-9:40	*Statistical Prediction of Crack Growth in a Tensioned Steel Band Using Transfer Mobilities, Mean Value Method, and Kalman Filtering,* D.C. Swanson	
9:40-10:05	*Chaotic Attractor Property Analysis In Vibration-Based Structural Damage Assessment,* M. Todd, J. Nichols, M. Seaver, S. Trickey, L. Pecora	
10:05-10:30	*Signal Diagnostics Applied to Engineering and Natural Dynamical Systems,* D.C. Lin, J. Thevaril	
10:30-10:55	*Detecting Measurement Noise in Chaotic Signals,* K. Hartt, D. Chelidze	
10:55-11:20	*Construction of Nonlinear Data-driven Models for Condition Monitoring and Calibration with a Review of an Application to Space Telescopes,* N.B. Tufillaro, D. Usikov, L. Barford, L. Marochnik, R. McCutheon	

MA6 Ballrm-D	*General Topics (24)*	Organizer: C.E. Bakis Chair: L.H. Friedman
9:15-9:40	*Non-Linear Electromechanically Coupled Modeling of Thin Piezoelastic Composite Plates,* M. Krommer	
9:40-10:05	*Optimal Spray Patterns For Liquid Application to Structured Packing,* S.C. Kranc	
10:05-10:30	*Thoughts on the use of Science Fiction in Engineering Instruction to Teach Basic Concepts and to Create Positive Images of the Profession,* A. Segall	
10:30-10:55	*TEM Investigation of Indentation Induced Phase Transformations in Silicon,* D. Ge, V. Domnich, Y. Gogotsi	
10:55-11:20	*Optimization of High Specific Power Electric Machines with Simulated Annealing,* A. Arvin, C. Bakis, H. Hofmann	

MA7 Ballroom-E	*Compliant Mechanisms (2)*	Organizers: M.I. Frecker, G.K. Ananthasuresh Chairs: M.I. Frecker, G.K. Ananthasuresh
9:15-9:40	*Topology Optimization of Compliant Mechanisms and Piezoelectric Actuators for Dynamic Applications.* M. Frecker, H. Maddisetty	
9:40-10:05	*High Authority Actuators.* H. Bart-Smith, D.R. Mumm, A.G. Evans, T.J. Lu	
10:05-10:30	*Alternate Modeling and Design Parameterization for the Topology Optimization of Compliant Mechanisms,* A. Saxena, L. Yin, N. Mankame, Z. Qian, G.K. Ananthasuresh	
10:30-10:55	*Optimal Embedding Approach to the Design of Heterogeneous Structures and Compliant Mechanisms,* Z. Qian, S.K. Koh, G.K. Ananthasuresh	

MA8 Mt. Nittany	*Active and Passive Models of Biological Tissue and Functional Engineered Tissue (1)*	Organizers: E.M. Arruda, K. Grosh Chairs: E.M. Arruda, K. Grosh
9:15-9:40	*Characterization of the Active and Passive Response of Self-Organized Cardiac Muscle Constructs,* R.G. Dennis, E.M. Arruda	
9:40-10:05	*A New Viscoelastic Anisotropic Model for Planar Collagenous Biomaterials,* J.E. Bischoff	
10:05-10:30	*Mechanical Models of Aneurysm Within the Framework of Hyperelasticity,* J.F. Ganghoffer, B. Haussy	
10:30-10:55	*Growth and Morphogenesis: A Continuum Field Theory,* K. Garikipati, E. Arruda, K. Grosh, S. Calve	

Concurrent Sessions — Monday B, 12:35–2:40 PM

MB1 Boardrm-1	*S. Nemat-Nasser Symposium (15)*	Organizers: J.R. Willis, M. Zikry Chairs: H.D. Espinosa and M. Hori
12:35-1:00	*Interfacial Microstructurally Induced Failure Modes,* M. Zikry, W. Ashmawi	
1:00-1:25	*Continuum and Atomistic Studies of Intersonic Crack Propagation,* Y.Huang	
1:25-1:50	*Micromechanics-based Continuum Model for Evaluation of Change in Permeability of Discontinuous Rock Due to Excavation of Nuclear Waste Disposal Tunnel,* H. Horii, J. Inoue, H. Kim, H. Yoshida	
1:50-2:15	*Asymptotic Models of Vibration of Elastic Structures in an Electro-Magnetic Field,* A. Movchan	
2:15-2:40	*Constitutive Modeling of Strain-Hardening Hyperelastic Materials,* C.O. Horgan, G. Saccomandi	

MB2 Fireside	*A.C. Eringen Symposium (7)*	Organizers: M.N.L. Narasimhan, A.D. Kirwan, Jr. Chair: T. Chang
12:35-1:00	*Forced and/or Self-Organized Criticality and Topological Phase Transitions in Space Plasmas,* T. Chang	
1:00-1:25	*Thermo-Mechanics of Materials as a Field Theory,* G.A. Maugin	
1:25-1:50	*Predictability, Uncertainty, and Hyperbolicity,* A.D. Kirwan, Jr., M. Toner, B. Lipphardt, Jr., L. Kantha	
1:50-2:15	*Wall Effects on a Spherical Particle,* H. Ramkissoon, R. Karim	
2:15-2:40	*A Thermodynamic Framework for Describing the Flows of Anisotropic Fluids,* K.R. Rajagopal	

MB3 Ballrm-A	*Dynamic Fracture (5)*	Organizers: F. Costanzo, J.R. Walton Chairs: F. Costanzo, J.R. Walton
12:35-1:00	*Interaction of Sound with Fast Crack Propagation,* S. Ciliberto	
1:00-1:25	*The Velocity Gap in Single-Crystal Silicon,* R.D. Deegan, M.P. Marder, H.L. Swinney	
1:25-1:50	*Velocity Gap in Silicon,* M. Marder	
1:50-2:15	*An Atomistic Study of Dynamic Brittle Fracture in Silicon,* J.G. Swadener, M.I. Baskes, M. Nastasi	
2:15-2:40	*Numerical and Experimental Investigations of Dynamic Interfacial Crack Growth in Composite-Homalite Bimaterials,* D. Coker, A. Needleman, A.J. Rosakis	

MB4 Ballrm-B	*Micro- and Nano-Scale Engineering (11)*	Organizer: T.J. Mackin Chair: T.J. Mackin
12:35-1:00	*Nanoengineering, Nanotribology, and MEMS: A Multi-Scale Approach to Controlling Friction and Wear,* R.W. Carpick, E.E. Flater, J.R. VanLangendon, J. Knapp, M.P. DeBoer	
1:00-1:25	*Mechanical Properties of Carbon-Nanotube/Al2O3 Composites,* Z. Xiu, W.A. Curtin, B. Sheldon, J. Xu, L. Reister	
1:25-1:50	*A Hybrid Continuum/Tight-Binding Analysis to Study the Effect of Mechanical Deformation on the Electrical Property of Carbon Nanotubes,* B. Liu, H.T. Johnson, H. Jiang, Y. Huang	
1:50-2:15	*Indentation of Freestanding Membranes With Finite Contact Sizes,* M.R. Begley, T.J. Mackin	
2:15-2:40	*Measurements of Polymer Viscoelasticity Using Depth-Sensing Indentation,* M.R. VanLandingham, C.C. White	

(more Monday B on next page)

Concurrent Sessions — Monday B, 12:35–2:40 PM

MB5 Boardrm-2	*Dynamical Systems Methods for Advanced Diagnostics and Prognostics (6)*	Organizers: J.P. Cusumano, D. Chelidze Chairs: J.P. Cusumano, D. Chelidze
12:35-1:00	*Vibration-based Damage Assessment Using Novel Function Statistics with Multiple Time Series,* L. Moniz, T. Carroll, L. Pecora, M. Todd, S. Trickey, J. Nichols	
1:00-1:25	*Fault Detection, Diagnosis and Prognosis of Bearings Using Hidden Markov Modeling of Vibration Signals,* H. Ocak, K.A. Loparo	
1:25-1:50	*Phase Space Warping: A General Approach to Machinery Diagnosis and Prognosis,* D. Chelidze, J.P. Cusumano	
1:50-2:15	*Model-Based Fault Detection and Diagnosis in Rotating Machinery,* K.A. Loparo, A. Fallah, M.L. Adams	
2:15-2:40	*Structural Damage Prognosis Using Nonlinear Dynamics,* M. Nataraju, D.E. Adams	

MB6 Ballrm-D	*Mechanics and Physics of Solid-Solid Phase Transformations (10)*	Organizers: D.C. Lagoudas, V.I. Levitas, I. Karaman Chairs: D.C. Lagoudas, V.I. Levitas, I. Karaman
12:35-1:00	*SMA Kinetics Characterization: Micromechanics to Continuum,* L.C. Brinson, D. Burton, X. Gao	
1:00-1:25	*Finite Element Modeling of Martensitic Transformation Based on Phase Field Theory,* A.V. Idesman, V.I. Levitas	
1:25-1:50	*An Absorbing Boundary Condition for 1-D Nonlinear Wave-Type Equations with Application to Impact Loading of Shape Memory Alloy Rods,* D.C. Lagoudas, A. Safjan, M. Newman, P. Popov	
1:50-2:15	*A Computational Study of Evolving Phase Fronts in Shape Memory Alloy Thin Films,* V. Stoilov, A. Bhattacharyya, J. Yokota	
2:15-2:40	*On the Multiaxial Mechanical Response of Polycrystalline NiTi Alloys,* P. Papadopoulos, R.O. Ritchie	

MB7 Ballrm-E	*Thermomechanics of the Inelastic Behavior of Materials (29)*	Organizers: A. Srinivasa, K.R. Rajagopal Chairs: A. Srinivasa, K.R. Rajagopal
12:35-1:00	*Thermomechanical Modeling of Dissipative Processes Utilizing a Framework with Multiple Natural Configurations,* K.R. Rajagopal	
1:00-1:25	*An Experimental Study of the Thermo-Mechanical Response of Elastomers Undergoing Scission and Cross-linking at High Temperatures,* A. Wineman, A. Jones, J. Shaw	
1:25-1:50	*On the Modeling of an Anisotropic Fluid within a Multiconfigurational Framework,* A.R. Srinivasa	
1:50-2:15	*Modeling Fiber Drawing Processes,* S. Bechtel	
2:15-2:40	*Analysis of the Film Casting Process Using a Continuum Model for Crystallization,* I.J. Rao, G.J. Barot	

MB8 Mt. Nittany	*Active and Passive Models of Biological Tissue and Functional Engineered Tissue (1)*	Organizers: E.M. Arruda, K. Grosh Chairs: E.M. Arruda, K. Grosh
12:35-1:00	*Can We Identify Vulnerable Plaques and the Location of Plaque Rupture with Numerical Methods?,* G.A. Holzapfel, Th.C. Gasser, Ch.A.J. Schulze-Bauer	
1:00-1:25	*Nonlinear Constitutive Laws for Cochlear Outer Hair Cells,* K. Grosh, J. Bischoff, E. Arruda, N. Deo	
1:25-1:50	*Piezoelectric-type Constitutive Relations for the Cochlear Outer Hair Cell,* A.A. Spector	
1:50-2:15	*Modeling the Effects of Restructuring on the Constitutive Response of Cervical Stroma,* S. Febvay, S. Socrate	
2:15-2:40	*Constitutive Modelling and Material Property Determination for the Collagen Network of Articular Cartilage,* V. Costanzo, S. Socrate, M.C. Boyce	

Concurrent Sessions — Monday C, 2:55–5:50 PM

MC1 Boardrm-1	*S. Nemat-Nasser Symposium (15)* Organizers: J.R. Willis, M. Zikry; Chairs: H. Horii and P. Ponte Castaneda
2:55-3:20	*Strain Localization Estimate in Plane Strain by Non-Coaxial Plasticity with Double Slip System,* T. Iwakuma
3:20-3:45	*Modeling Damage with Shear Bands and Voids in Metals,* T.W. Wright, S. Schoenfeld, K.T. Ramesh, X.Y. Wu
3:45-4:10	*Ductile Fracture: Modeling, Simulation, and Experiments,* M.M. Rashid
4:10-4:35	*Characterization of Ductile and Brittle Modes of Material Removal using Single-Grit Scratching,* G. Subhash, J.E. Loukus, S.S. Pandit
4:35-5:00	*Elasticity, Plasticity and Fracture of Thin Films and MEMS Materials: Size Effects in Submicron Gold Films,* H.D. Espinosa, B.C. Prorok

MC2 Fireside	*A.C. Eringen Symposium (7)* Organizers: M.N.L. Narasimhan, A.D. Kirwan, Jr.; Chair: J.D. Lee
2:55-3:20	*The Hydrodynamics of Liquid Crystal with Magnetic and Electric Fields,* M.-C.T. Calderer, C. Liu
3:20-3:45	*Modeling of Ferroelectric Liquid Crystals,* C. Liu, M.-C.T. Calderer
3:45-4:10	*On Forces and Applications in MicroElectroMechanical Systems,* S.-A. Zhou
4:10-4:35	*New Concepts in Nonlocal Mechanics and New Materials Obeying a Generalized Continuum Behavior,* J.F. Ganghoffer
4:35-5:00	*Application of Nonlocal Continuum Models to Nanotechnology,* J. Peddieson, G.R. Buchanan, R.P. McNitt

MC3 Ballrm-A	*Dynamic Fracture (5)* Organizers: F. Costanzo, J.R. Walton; Chairs: F. Costanzo, J.R. Walton
2:55-3:20	*Dynamic Steady-State Crack Propagation in an Anisotropic Linear Viscoelastic Body,* J.R. Walton
3:20-3:45	*A Dynamically Accelerating Semi-Infinite Crack in a Linear Viscoelastic Material,* T.L. Leise, J.R. Walton
3:45-4:10	*3D Simulations for Dynamic Crack Propagation in Brittle Materials Using Rate-Dependent Cohesive Models,* F. Zhou, J.-F. Molinari
4:10-4:35	*On the Use of Space-time Finite Element Method in the Solution of Dynamic Crack Propagation,* H. Huang, F. Costanzo
4:35-5:00	*Stress Waves and Cohesive Failure in a Finite Strip Subjected to Transient Loading,* G.A. Gazonas, D.H. Allen
5:00-5:25	*Experimental Verification and Validation of Virtual Internal Bond Model Parameters for Simulating Dynamic Crack Behavior,* G. Thiagarajan, J.K. Hsia, Y.Y. Huang

MC4 Ballrm-B	*Micro- and Nano-Scale Engineering (11)* Organizer: T.J. Mackin; Chair: T.J. Mackin
2:55-3:20	*Mechanical Characterization of Ultra Thin Nano-Crystalline Metal Films by MEMS Instruments,* T. Saif, A. Haque
3:20-3:45	*Thermomechanical Model Predictions for the Response of Adhered MEMS Cantilevers Due to Laser Heating,* J.W. Rogers, T.J. Mackin, L.M. Phinney
3:45-4:10	*Mechanical and Constitutive Properties of Thin, Soft Layers: Preliminary AFM Experiments and Related Modeling,* E.J. Berger, K. Vemaganti, L. Yu, H. You
4:10-4:35	*Static Dielectric Constant of Particulates Determined with Electroacoustic and Attenuation Spectroscopy,* T. Hao, V. Atakan, R.E.Riman
4:35-5:00	*Nanostructured Alumina Coating on Aluminum or Alloys,* M. Kireitseu, I. Nemerenco, L. Yerakhavets

(more Monday C on next page)

Concurrent Sessions — Monday C, 2:55–5:50 PM

MC5 Brdrm-2	*Dynamical Systems Methods for Advanced Diagnostics and Prognostics (6)*	Organizers: J.P. Cusumano, D. Chelidze Chairs: J.P. Cusumano, D. Chelidze
2:55-3:20	*Karhunen-Loeve Based Order Reduction of Dynamics of Flexible Structures with Application to System Modelling and Diagnosis/Prognosis of Faults,* A. Vakakis, L. Bergman, X. Ma	
3:20-3:45	*Assessment of the Robustness of the Neuro-Fuzzy Forecasting System,* W. Wang, F. Golnaraghi, F. Ismail	
3:45-4:10	*Screening of Human Movement Disorders: Use of Dynamical Analyses in Distinguishing between Aging and Disease,* K.M. Newell, D.E. Vaillancourt	
4:10-4:35	*Hidden Variable Tracking for Monitoring Long-Term Changes in Human Coordination,* J.B. Dingwell	
4:35-5:00	*Discrete and Rhythmic Dynamics as Units of Coordinated Action: Behavioral Data, a Dynamic Model, and Brain Imaging Results,* D. Sternad	
5:00-5:25	*Changes in Foot Loading Following Plantar Fasciotomy: A Computer Modeling Study,* A. Erdemir, S.J. Piazza	

MC6 Ballrm-D	*Mechanics and Physics of Solid-Solid Phase Transformations (10)*	Organizers: D.C. Lagoudas, V.I. Levitas, I. Karaman Chairs: D.C. Lagoudas, V.I. Levitas, I. Karaman
2:55-3:20	*Thermal and Mechanical Characteristics of Ti-Rich NiTi Processed by ECAE at Different Temperatures,* H.E. Karaca, I. Karaman, Z. Luo	
3:20-3:45	*Active Skin for Turbulent Drag Reduction,* R. Mani, D.C. Lagoudas, O.K. Rediniotis	
3:45-4:10	*Evolution of Ferroelectric Domain Structures in Thin Film with Structural Defects,* S. Hu, Y. Li, L. Chen	
4:10-4:35	*Energy Minimization, Microstructure and Effective Behavior of Phase Transforming Materials,* I.V. Chenchiah, K. Bhattacharya	
4:35-5:00	*Three-dimensional Landau Theory for Multivariant Stress-induced Martensitic Phase Transformations,* V.I. Levitas, D.L. Preston	
5:00-5:25	*Modeling and Simulation of Phase Transformations in Materials,* T. Cagin	
5:25-5:50	*Multiscale Modeling of Strain-Induced Phase Transformations under High Pressure,* V.I. Levitas	

MC7 Ballrm-E	*Thermomechanics of the Inelastic Behavior of Materials (29)*	Organizers: A. Srinivasa, K.R. Rajagopal Chairs: A. Srinivasa, K.R. Rajagopal
2:55-3:20	*A Simple Model for the Effective Thermal Conductivity of Granular Materials,* M. Massoudi, T.X. Phuoc	
3:20-3:45	*On Creep-Fatigue Interactions in Metals,* G. Rengarajan	
3:45-4:10	*A Computational Framework for Consistent Embedding of Scales Arising in Multiscale Modeling of Materials,* A. Masud	
4:10-4:35	*Common Trends in Deformation of Low Stacking Fault Energy Austenitic Steels,* I. Karaman, H. Sehitoglu, H. Meier, Y.I. Chumlyakov, I. Kireeva	
4:35-5:00	*Coupled Field Formulations for Mechanics and Diffusion in Crystalline,* K. Garikipati	
5:00-5:25	*A Damage Mechanics Theory Without a Potential Surface,* C. Basaran	
5:25-5:50	*Constitutive Modeling of Asphalt Concrete,* M. Krishnan	

MC8 MtNittany	*Cell and Molecular Bioengineering (30)*	Organizers: P.J. Butler, C. Dong Chairs: P.J. Butler, C. Dong
2:55-3:20	*Mechanosensing Via Membrane-lipid Perturbations,* P.J. Butler, S. Chien, B.P. Bowen, N. Woodbury	
3:20-3:45	*Bone Cell Mechanobiology,* H.J. Donahue, C.R. Jacobs, Z. Li, M.M. Saunders, C.E. Yellowley, J. You, Z. Zhou	
3:45-4:10	*Strategies for Microneedle Enhanced Drug Delivery and Biomedical Sensing,* J.D. Zahn, A.P. Pisano, D. Liepmann	
4:10-4:35	*Side-view Imaging and Analysis of Cell Adhesion to ICAM-1 in Shear Flow,* C. Dong	
4:35-5:00	*Submolecular Changes in Fibrinogen Conformation on Model Biomaterial Surfaces,* C. Siedlecki, A. Agnihotri	
5:00-5:25	*Harnessing Kinesin Motor Proteins for Force Generation and Nanoscale Transport Along Immobilized Microtubule Tracks,* W.O. Hancock	

Concurrent Sessions — Tuesday A, 9:15–11:20 AM

TA1 Boardrm-1	*S. Nemat-Nasser Symposium (15)*	Organizers: J.R. Willis, M. Zikry Chairs: M.M. Rashid and G. Subhash
9:15-9:40	*Inversion of Stress Tensor using Integrated Photoelasticity,* M. Hori, K. Oguni, W.L.L. Wijerathne	
9:40-10:05	*Stress Analysis of an Undulated Plate by the Combined First Order Perturbation and Alternating Method,* Y. Sumi, A. Rahbar-Ranji	
10:05-10:30	*Bounding the Stress-Strain Response of a Nonlinear Composite,* J.R. Willis	

TA2 Fireside	*A.C. Eringen Symposium (7)*	Organizers: M.N.L. Narasimhan, A.D. Kirwan, Jr. Chair: G. Maugin
9:15-9:40	*Constitutive Relations of Micromorphic Thermoplasticity,* J.D. Lee, Y. Chen	
9:40-10:05	*On Multiple Routes to Chaos in Advection Induced by Point Vortices,* I. Kunin, F. Hussain, X. Zhou	
10:05-10:30	*The Contributions of Microrotation of Lubricant Molecules in a Journal Bearing,* R.S.R. Gorla	
10:30-10:55	*Discrete Systems of Controlled Pendulum Type,* B. Yamrom, I. Kunin, R. Metcalfe, G. Chernykh	
10:55-11:20	*Lorenz-Type Controlled Pendulum,* I. Kunin, B. Kunin	

TA3 Ballrm-A	*Student Paper Competition (18)*	Organizers: W. Thompson, Jr., C.E. Bakis Chair: W. Thompson, Jr.
9:15-9:40	*Finite Strain Response and Texture Evolution of alpha- and beta-Crystalline Polypropylene,* W. Xu, E.M. Arruda	
9:40-10:05	*Thermodynamic Framework for Coupling of Non-Local Viscoplasticity and Non-Local Anisotropic Viscodamage for Dynamic Localization Problems Using Gradient Theory,* R.K. Abu Al-Rub, G.Z. Voyiadjis, A.N. Palazotto	
10:05-10:30	*Strain Rate Sensitivity of Cymat Aluminum Foam Subject to Uniaxial Compressive Loading,* M.M. Braun, K.A. Issen	
10:30-10:55	*Experimental Analysis of Compaction Band Formation in Aluminum Foam Using Surface Strain Mapping,* T.P. Casey, K.A. Issen	
10:55-11:20	*Tissue Engineering and Characterization of Self-Organized Tendon Constructs,* S. Calve, R.G. Dennis, K. Grosh, E.M. Arruda	

TA4 Ballrm-B	*Wear and Tribology (22)*	Organizers: A.E. Segall, J.C. Conway Chair: A.E. Segall
9:15-9:40	*Frictional and Adhesive Properties of Diamond-like Carbon at the Nano Scale,* R.W. Carpick, E.E. Flater, J.R. VanLangendon, K. Sridharan	
9:40-10:05	*The Effects of Ion Implantation of Nitrogen and Boron on the Wear Resistance of W18Cr4V Steel,* P. Zhang, Z. Liang, Z. Hu, D. Liu	
10:05-10:30	*Coatings for Anti-Fretting Behavior: Tribochemistry at Fretted Interfaces,* J.H. Sanders, S.K. Sharma, C.H. Hager, Jr., T.C. Back	
10:30-10:55	*Tribological Properties of Nanostructured Carbide-Derived Carbons,* Y. Gogotsi, B. Carroll, A. Kovalchenko, A. Erdemir, M.J. McNallan	
10:55-11:20	*Failure Mechanism of Ceramic Coatings in Load Limited Scratch Tests,* I. Shareef, L. Ajayi, G. Fenske	

(more Tuesday A on next page)

Concurrent Sessions — Tuesday A, 9:15–11:20 AM

TA5 Boardrm-2	*Quantum/Atomistic/Continuum Coupling in Materials Simulation (16)*	Organizers: H.T. Johnson, W.A. Curtin Chairs: H.T. Johnson, W.A. Curtin
9:15-9:40	*Connecting Atomistics to Continuum Elasticity: Modeling Vacancies in Stillinger-Weber Silicon,* M. Bouville, D. de Graeve, M. Falk, K. Garikipati	
9:40-10:05	*Atomistic and Continuum Analysis of Residual Stress Effects in an Ion-Beam Machined Thin Film MEMS Structure,* H.T. Johnson, M.C. Moore, J.B. Freund, T.G. Bifano	
10:05-10:30	*Dynamically Equivalent Continuum Interpretation of Discrete Molecular Behavior at Arbitrary Scales,* M. Zhou	
10:30-10:55	*Mechanics of Carbon Nanotubes: A Continuum Analysis Incorporating the Interatomic Potentials,* Y. Huang, P. Zheng, H. Jiang, B. Liu, H.T. Johnson	
10:55-11:20	*Nonlocal Separation Constitutive Laws for Interfaces Informed by Nano-Scale Simulations,* D.E. Spearot, K.I. Jacob, D.L. McDowell	

TA6 Ballrm-D	*Structural Dynamics and Stability (28)*	Organizers: E. Mockensturm, A. Raman Chairs: E. Mockensturm, A. Raman
9:15-9:40	*Equilibrium and Belt-Pulley Vibration Coupling in Serpentine Belt Drives,* L. Kong, R. Parker	
9:40-10:05	*Secondary Buckling and Tertiary States in a Beam on a Nonlinear Elastic Foundation,* K. Murphy, Y. Zhang	
10:05-10:30	*Nonresonant Modal Interactions in a Flexible Externally Excited Cantilever Beam,* P. Malatkar, A.H. Nayfeh	
10:30-10:55	*An Embedded Sensitivity Approach for Diagnosing System-Level Noise and Vibration Problems,* C. Yang, D.E. Adams, S.-W. Yoo, H.-J. Kim	
10:55-11:20	*A Theoretical and Experimental Investigation of the Global Dynamics of Buckled Beams,* S.A. Emam, A.H. Nayfeh	

TA7 Ballrm-E	*Thermo-Mechanical Problems (20)*	Organizers: P. Michaleris, N. Zabaras Chairs: P. Michaleris, N. Zabaras
9:15-9:40	*Computational Design of Multi-stage Deformation Processes,* N. Zabaras, S. Ganapathysubramanian	
9:40-10:05	*A Transient Thermal Tensioning Process for Mitigating Distortion in Stiffened Structures,* J.Y. Shanghvi, J.R. Dydo	
10:05-10:30	*3-D Fracture Analysis of I-Beams with Fillet Welds,* E. Citirik, H.F. Nied	
10:30-10:55	*Sensitivity Analysis and Optimization of the Thermo-Elasto-Plastic Process with Applications to Welding Side Heater Design,* J. Song, P. Michaleris	
10:55-11:20	*Coupled Solid State Diffusion and Mechanics in a Field Formulation,* K. Garikipati	

TA8 Mt. Nittany	*Synergistic Enviro-Mechanical Degradation Kinetics and Acceleration (19)*	Organizers: J.J. Lesko, A. Szekeres Chairs: J.J. Lesko, A. Szekeres
9:15-9:40	*Strength and Durability of Graphite/Epoxy Composites Under Hygrothermal Conditions,* S.R. Patel, S.W. Case	
9:40-10:05	*Mechanical Behavior of Center-Hole Notched Nicalon/Silicon Carbide Ceramic Composites,* H.G. Halverson, S.W. Case	
10:05-10:30	*Hygrothermal Effects of Deionized Water and Alkaline Solutions on Durability of Pultruded E-Glass/Vinylester Composites,* W. Chu, V.M. Karbhari	
10:30-10:55	*Synergistic Effects of Aqueous Immersion, Temperature and Stress on Durability of Ambient Composites Cured Under Ambient Conditions,* V.M. Karbhari, C. Helbling, Y. Li	
10:55-11:20	*Development of Service Life Prediction & Accelerated Aging Methodologies for Glass/Thermosetting Composites,* N. Verghese, L. Blankenship, J. Lesko	
11:20-11:45	*Moisture Absorption and Strength Characterization of Hygrothermally Aged Pultruded Vinyl Ester E-Glass Laminates,* S. Phifer, J. Lesko	

Concurrent Sessions — Tuesday B, 12:35–2:40 PM

TB1 Boardrm-1	*Particle Systems — Measurement Methods and Constitutive Models (13)*	Organizers: V.M. Puri, J.G. Arguello Chairs: V.M. Puri, J.G. Arguello
12:35-1:00	*Anisotropy in Powder Compaction: Methods for Analysis and Testing,* A.L. Gurson	
1:00-1:25	*Properties of Granulated Ceramic Powders in Hydrostatic and Triaxial Compression,* D.H. Zeuch, J.M. Grazier, J.G. Arguello, K.G. Ewsuk	
1:25-1:50	*Quantification and Constitutive Modeling of Visco-elastoplastic Properties of Ceramic Powders Using a Cubical Triaxial Tester,* B. Mittal, V.M. Puri	
1:50-2:15	*Deformation Characteristics of a Single Alumina Granule under a Normal Compressive Load,* I. Aydin, M.A. Gurkaynak	
2:15-2:40	*Investigating Axial and Radial Powder Movements during the Compaction of Pharmaceutical Excipients,* B. Eiliazadeh, B.J. Briscoe, K. Pitt	

TB2 Fireside	*A.C. Eringen Symposium (7)*	Organizers: M.N.L. Narasimhan, A.D. Kirwan, Jr. Chair: S. Nemat-Nasser
12:35-1:00	*Statistical Mechanics and 3-Camera, 3D, Particle-Tracking Velocimetry Studies of Anomalous Dispersion,* J.H. Cushman, M. Moroni, A. Cenedese	
1:00-1:25	*Length-Scale in Plasticity,* S. Nemat-Nasser	
1:25-1:50	*On Extracting Physical Information from Mathematical Models of Chaotic and Complex Systems,* I. Kunin	
1:50-2:15	*Surface Cracking of Graded Materials Due to Sliding Contact,* F. Erdogan, S. Dag	

TB3 Ballrm-A	*Student Paper Competition (18)*	Organizers: W. Thompson, Jr., C.E. Bakis Chair: W. Thompson, Jr.
12:35-1:00	*Conditions for Localized Compaction in High Porosity Sandstone,* V. Challa	
1:00-1:25	*Low K Dielectric Thin Film Development and High Frequency Characterization,* H.-P. Hsueh, M.T. Lanagan, R.T. McGrath	
1:25-1:50	*Tool Condition Monitoring,* S. Jayasankar	
1:50-2:15	*Nanoindentation of Alumina Matrix - Chrome Carbide Nanoparticles Composite,* L. Yerakhavets, M. Kireitseu, I. Nemerenco	
2:15-2:40	*Rheological Behavior and Model of Alumina-Polymer-Based Composites,* I. Nemerenco, M. Kireitseu, L. Yerakhavets	

TB4 Ballrm-B	*Wear and Tribology (22)*	Organizers: A.E. Segall, J.C. Conway Chairs: J. Perez
12:35-1:00	*Temperature-Dependent Degradation Mechanisms in Cu-Ni-In Anti-Fretting Coatings and the Complicated Search for Alternatives,* A. Segall, J. Conway, Jr., C. Hager	
1:00-1:25	*Handheld Slipmeter to Measure Slip Resistance between Shoe and Flooring Materials,* H.J. Sommer III, J.J. Stauffer	
1:25-1:50	*Measurement of Interfacial Wear using Focused Ion Beam Milling,* J. Kiely, Y.-T. Hsia, T. Clinton	
1:50-2:15	*Micromechanical Modeling of Contact/Friction in Ceramic Materials Under Pressure-Shear Loading,* H.D. Espinosa, P.D. Zavattieri, S.S. Lee	
2:15-2:40	*Simulating the Contact and Interaction of Engineering Surfaces,* Q.J. Wang, S. Liu	

(more Tuesday B on next page)

Concurrent Sessions — Tuesday B, 12:35–2:40 PM

TB5 Boardrm-2	*Quantum/Atomistic/Continuum Coupling in Materials Simulation (16)*	Organizers: H.T. Johnson, W.A. Curtin Chairs: H.T. Johnson, W.A. Curtin
12:35-1:00	*Evolution of the Dislocation Core Structure During Dislocation Glide in an FCC Lattice,* R.C. Picu, M.A. Soare	
1:00-1:25	*Dislocation Motion in Al-Mg: Computer Simulations of Solid Solution Hardening,* D.L. Olmsted, W.A. Curtin, R.J. Clifton, L.G. Hector, Jr.	
1:25-1:50	*A Stress-Gradient Based Criterion for Dislocation Nucleation in Crystals: Theory and Simulation,* R.E. Miller, A. Acharya	
1:50-2:15	*Phase Field Modelling of the Portevin-Le Chatelier Effect from the Dynamic Drag of Solute Atmosphere,* S. Hu, J. Choi, L. Chen	

TB6 Ballrm-D	*Structural Dynamics and Stability (28)*	Organizers: E. Mockensturm, A. Raman Chairs: E. Mockensturm, A. Raman
12:35-1:00	*Nonlinear Modeling and Dynamic Stability of a Uniformly Loaded Thin, Rotating, Circular Disk,* A. Renshaw	
1:00-1:25	*Instability Mechanisms of a Supercritical Flexible Disk Rotating in an Acoustic Cavity,* N. Kang, A. Raman	
1:25-1:50	*Combination Parametric Resonance of Nonlinear Circular Plate Subjected to Thermal Loading,* W.F. Faris, A.H. Nayfeh	
1:50-2:15	*Vibration of Flex Circuits in Hard Disk Drives,* J. Wickert	
2:15-2:40	*Stability of a Supercritical Driveline Connected by Non-Constant Velocity Couplings Subjected to Misalignment and Torque,* H.A. Desmidt, K.W. Wang, E.C. Smith	

TB7 Ballrm-E	*Thermo-Mechanical Problems (20)*	Organizers: P. Michaleris, N. Zabaras Chairs: P. Michaleris, N. Zabaras
12:35-1:00	*Development of Inhomogeneous Response in an Elastomeric Component Due to Thermally Induced Scission and Healing,* A.S. Wineman, J.-H. Min	
1:00-1:25	*Thermal Fields Caused by Point Sources in Multiply-Connected Inhomogeneous Regions,* Y.A. Melnikov	
1:25-1:50	*Implementation of Eulerian Finite Element Formulation on Modeling Laser Forming,* L. Zhang, P. Michaleris	

TB8 Mt. Nittany	*Growth in Biological Tissues (9)*	Organizers: I.J. Rao, G. Praveen Chairs: I.J. Rao, G. Praveen
12:35-1:00	*Heterogeneity in Myocardial Structure Correlates Well with Heterogeneity in the Strain Field,* J.C. Criscione	
1:00-1:25	*A Constrained Mixture Model for Biological Growth and Remodeling,* I.J. Rao, J.D. Humphrey, K.R. Rajagopal	
1:25-1:50	*Thermo-Mechanical Degradation of Rubber: Mechanical Consequences and Implications for Soft Tissue Modeling,* A. Wineman, K. Myers	

Concurrent Sessions — Tuesday C, 2:55–5:00 PM

TC1 Boardrm-1	*Particle Systems — Computational Methods (13)*	Organizers: V.M. Puri, J.G. Arguello Chairs: J.G. Arguello, V.M. Puri
2:55-3:20	*Dynamic Behavior of an Intruder in Boundary-Driven Granular Flows,* J. Liu, A.D. Rosato, D.L. Blackmore	
3:20-3:45	*Maximum Packing Fraction Predicted on the Basis of Particle Size Distribution and Determined via the Rheological Measurement,* T. Hao, R.E. Riman	
3:45-4:10	*Continuum-Based FEM Modeling of Ceramic Powder Compaction,* J.G. Arguello, A.F. Fossum, D.H. Zeuch, K.G. Ewsuk	
4:10-4:35	*A Finite Element Study of Particle Fragmentation During Compaction of Particulate Materials,* A. Zavaliangos	
4:35-5:00	*Simulation of the Die Compaction and Sintering Process with Finite Element Method,* R. Zhang, Y.-S. Kwon, R.S. Engel, N.J. Salamon	

TC2 Fireside	*A.C. Eringen Symposium (7)*	Organizers: M.N.L. Narasimhan, A.D. Kirwan, Jr. Chair: I.A. Kunin
2:55-3:20	*Kolmogorov Complexity and Chaotic Phenomenon,* V. Kreinovich, I. Kunin	
3:20-3:45	*Method of Algorithmic Transformations with Applications to Chaotic Systems,* B. Yamrom, I.A. Kunin, G.A. Chernykh	
3:45-4:10	*A New Geometrical Approach to Chaos,* S. Preston, I. Kunin, J. Gliklikh	
4:10-4:35	*Centroidal Trajectories and Frames for Chaotic Dynamical Systems,* B. Yamrom, I.A. Kunin, G.A. Chernykh	
4:35-5:00	*Size Dependent Material Behavior at the Micron and Sub-micron Scales,* Y.Y. Huang	

TC3 Ballrm-A	*Simulation Based Control (17)*	Organizers: R.A. Wysk, Y.-J. Son Chairs: R.A. Wysk, Y.-J. Son
2:55-3:20	*A Bidding-Based Control Framework for a Random Flexible Manufacturing System with Alternate Routings,* T. Siwamogsatham, C. Saygin	
3:20-3:45	*A Federation Object Coordinator for Simulation Based Shop Floor Control and Analysis,* S. Lee, S. Ramakrishnan, R.A. Wysk	
3:45-4:10	*Simulation-based Control for an Automated Workstation,* J.S. Smith, A. Pai	
4:10-4:35	*Real-time Adaptive Shop Floor Control System: Using Simulation, Dispatching Rules, and Direct Search Algorithm,* M. Madan, P. Vijayakumar, J. Venkateswaran, Y.-J. Son	
4:35-5:00	*Tool Management in Flexible Manufacturing Systems: A Simulation Study,* N. Buyurgan, C. Saygin	

TC4 Ballrm-B	*Wear and Tribology (22)*	Organizers: A.E. Segall, J.C. Conway Chairs: W. Lloyd
2:55-3:20	*Wear Evaluation of HIP Compacted, Nitrogen Enhanced, Atomized Stainless Steels,* J.C. Rawers, F. Biancannielo	
3:20-3:45	*The Influence of Manufacturing Processes on the Reciprocating Wear Behavior of Hypereutectic B390 Alloys,* A. Segall, C. Hager, Jr., J. Conway, Jr., M.F. Amateau	
3:45-4:10	*A Study of Friction and Wear of Used Diesel Engine Oils,* J. Perez, E. Tersine, W. Lloyd	
4:10-4:35	*Friction and Wear of Some Vegetable Oil Based Lubricants,* J. Perez, K. Wain, K. Cheenkachorn, W. Lloyd	

(more Tuesday C on next page)

Concurrent Sessions — Tuesday C, 2:55–5:00 PM

TC5 Boardrm-2	*Quantum/Atomistic/Continuum Coupling in Materials Simulation (16)*	Organizers: H.T. Johnson, W.A. Curtin Chairs: H.T. Johnson, W.A. Curtin
2:55-3:20	*Multiscale Modeling of Plasticity in Dynamic Fracture of Ductile Metals,* R.E. Rudd, J. Belak, E.T. Seppala, M.C. Fivel	
3:20-3:45	*A Superposition Framework for Discrete Dislocation Plasticity,* M.P. O'Day, W.A. Curtin	
3:45-4:10	*Multiscale Modeling of 3D Polycrystals,* R. Radovitzky, A.M. Cuitino	
4:10-4:35	*Couple Stresses in Crystalline Solids: Origins from Plastic Slip Gradients, Dislocation Core Distortions, and Three-Body Interatomic Potentials,* K. Garikipati	

TC6 Ballrm-D	*Structural Dynamics and Stability (28)*	Organizers: E. Mockensturm, A. Raman Chairs: E. Mockensturm, A. Raman
2:55-3:20	*Large Electroelastic Deformation of an Axisymmetric Dielectric Membrane,* N. Goulbourne, E. Mockensturm, M. Frecker, A. Snyder	
3:20-3:45	*Dynamic Creep Buckling of Viscoelastic Columns with Large Deformations and Follower Loads - Failure Probabilities and Survival Times,* H.H. Hilton, M. Achour	
3:45-4:10	*When Does a Wrinkle Become a Crease?,* T. Scott, E. Mockensturm	
4:10-4:35	*Steady-Sliding Instability in Fiber Pullout Experiments: Stick-Slip Dynamics of a Two-Sided Contact,* E.J. Berger, T.J. Mackin	

TC7 Ballrm-E	*General Topics (24)*	Organizer: C.E. Bakis Chair: L.H. Friedman
2:55-3:20	*Gantry Cranes Gain Scheduling Control with Friction Compensation,* H.M. Omar, A.H. Nayfeh	
3:20-3:45	*Fatigue Crack Initiation in Pressure Vessels,* S. Chattopadhyay	
3:45-4:10	*The Influence of Broken Fiber Modulus and Slipping Yarn Friction on Stress Concentration in Hybrid Yarns,* J.N. Rossettos, T.A. Godfrey	
4:10-4:35	*Variation of Pressure Gradient Ratio in Dense Phase Pneumatic Transport Systems,* B.K. Datta, C. Ratnayaka	

TC8 Mt. Nittany	*Materials Modeling Issues for Engineering Systems (27)*	Organizers: D. Lo, B. Scherzinger Chairs: D. Lo, B. Scherzinger
2:55-3:20	*The Adhesion Behavior and Fundamentals of Alumina-based Ceramic Coatings and Nanostructures,* M. Kireitseu, I. Nemerenco, L. Yerakhavets	
3:20-3:45	*Nucleation and Propagation of an Edge Crack in a Uniformly Cooled Epoxy/Glass Bimaterial,* E.D. Reedy, T.R. Guess	
3:45-4:10	*Constitutive Restrictions for a New Class of Models Describing Isotropic, Nonlinearly Hyperelastic Materials,* J.P. Wilber, J. Criscione	
4:10-4:35	*A Dilatational Plasticity Theory for Viscoplastic Materials,* B. Chen, Y. Huang, C. Liu, P.D. Wu, S.R. MacEwen	
4:35-5:00	*Challenges in Modeling the Resistance Welding Process,* A.R. Ortega, J.W. Foulk III, M.L. Chiesa, D.K. Gartling	

Concurrent Sessions — Wednesday A, 9:15–11:20 AM

WA1 Boardrm-1	*Particle Systems — Modeling Methods (13)*	Organizers: V.M. Puri, J.G. Arguello Chairs: V.M. Puri, J.G. Arguello
9:15-9:40	*Experimental, Simulation and Nonlinear Dynamics Analysis of Galton's Board,* A.D. Rosato, D.L. Blackmore, L. Buckley, M. Johnson, C. Oshman	
9:40-10:05	*A Variographic Approch to Continuous Mixing of Particulate Material,* A. Ghaderi	
10:05-10:30	*Modeling the Dynamics of Fabric in a Rotating Horizontal Drum using the Discrete Element Method,* J. Park, C. Wassgren	
10:30-10:55	*A Parametric Pressing Study Using A Plastic-Bonded Explosive,* S.J. Powell, B.W. Olinger, L.R. Maez, D.J. Hayden	
10:55-11:20	*Vibration-Induced Densification of Granular Materials,* N. Zhang, A.D. Rosato	

WA2 Fireside	*Ultrasonic NDE (21)*	Organizers: J.L. Rose, C. Miyasaka Chairs: J.L. Rose, C. Miyasaka
9:15-9:40	*Singular Solution of an Integro-Differential Equation in Elastodynamics,* A.R. Aguiar, Y.C. Angel	
9:40-10:05	*Phenomenally High Transduction Piezoelectric Transducers and Introduction of Non-contact Ultrasound Analysis,* M.C. Bhardwaj	
10:05-10:30	*A Novel Technique with Magnetostrictive Transducers for Dimensional Analysis of a Distant Specimen,* M. Heckman, K. Oliver, M. Pedrick	
10:30-10:55	*Thermal Deformation of Alumina (Al_2O_3) Substrate During Soldering,* B. Bond	
10:55-11:20	*Investigation of Ultrasonic Characterization of Elastomers by Non-contact and Air-coupled Ultrasonic Technique,* K. Yu	

WA3 Ballrm-A	*Continuum Plasticity and Damage Mechanics (3)*	Organizers: C.J. Lissenden, G.Z. Voyiadjis Chairs: C.J. Lissenden, G.Z. Voyiadjis
9:15-9:40	*A Multiscale Gradient Theory for Elastoviscoplasticity of Single Crystals,* J.D. Clayton, D.J. Bammann, D.L. McDowell	
9:40-10:05	*A Higher-order Single Crystal Plasticity Model for Microscopic Length Scales,* A. Arsenlis, R. Becker, V.V. Bulatov, D.M. Parks	
10:05-10:30	*A Rational Mechanics Approach to Viscoelastic Fracture,* D.H. Allen, C.R. Searcy	
10:30-10:55	*On the Coupling of Damage and Plasticity Models for Ductile Materials,* G.Z. Voyiadjis, R. Abu Al-Rub	
10:55-11:20	*Experimentally Constructed Yield Surfaces for Reinforced Aluminum,* X. Lei, C. Lissenden	

WA4 Ballrm-B	*Wear and Tribology (22)*	Organizers: A.E. Segall, J.C. Conway Chairs: J.C. Rawers
9:15-9:40	*Lubrication Issues in Aircraft Hydraulic Pumps,* S.K. Sharma	
9:40-10:05	*Effects of Surface Modification on Thrust Washer Lubrication,* N. Bolander, F. Sadeghi, C. Wassgren	
10:05-10:30	*Advanced WC-Co Composites for Cutting Tool Applications,* K.M. Fox, J.R. Hellmann, M.F. Amateau, P.H. Cohen, B. Singh, W.-E. Fu	
10:30-10:55	*Experimental Investigation of the Effects of Feed and Speed on Exit Burr Formation in Drilling,* I. Abu-Mahfouz	

(more Wednesday A on next page)

Concurrent Sessions — Wednesday A, 9:15–11:20 AM

WA5 Boardrm-2	*Quantum/Atomistic/Continuum Coupling in Materials Simulation (16)*	Organizers: H.T. Johnson, W.A. Curtin Chairs: H.T. Johnson, W.A. Curtin
9:15-9:40	*Quantum-Atomistic Study of Interdiffusion in Si/Si1-xGex Multilayer Structures,* P. Ramanarayanan, K. Cho	
9:40-10:05	*Self-Assembly of Steps and Nanostructures on Si(113) Surfaces,* C.V. Ciobanu, V.B. Shenoy, C.Z. Wang, K.M. Ho	
10:05-10:30	*Flexible First-Principles Boundary Conditions: Simulating Isolated Dislocations in Metals,* C. Woodward, S.I. Rao	
10:30-10:55	*From Quantum-Mechanics to Fracture: Atomistics Multiscale Simulations of Silicon,* N. Bernstein	

WA6 Ballrm-D	*X-ray Computed Tomography in Materials Science & Engineering (23)*	Organizers: N.L. Rupert, J.M. Wells Chairs: N.L. Rupert, J.M. Wells
9:15-9:40	*High Resolution X-Ray Tomography for Micro-Analysis,* A. Simionovici, A. Somogyi, C. Rau, B. Golosio, M. Chukalina	
9:40-10:05	*Image Processing and Visualization of X-ray Computed Tomography Data,* W.H. Green, N.L. Rupert, J.M. Wells	
10:05-10:30	*Computed Tomography at the Air Force Research Laboratory,* C.V. Kropas-Hughes, C.D. Daniels, E.L. Klosterman	
10:30-10:55	*Comparison of Optical Coherence Tomography, X-Ray Computed Tomography and Confocal Microscopy Results from an Impact Damaged Epoxy/E-glass Composite,* R.S. Parnas, J.P. Dunkers, D.P. Sanders, D.L. Hunston, M.J. Everett, W.H. Green	
10:55-11:20	*The Detection of Porosity and Defects in Composite and Metal Samples with High Resolution Volumetric Computed Tomography,* F. Hopkins, Y. Du, W. Ross, S. Basu	

WA7 Ballrm-E	*Multiscale Modeling of Solidification (25)*	Organizers: M.F. Horstemeyer, D.B. Kothe Chairs: M.F. Horstemeyer, D.B. Kothe
9:15-9:40	*Computing Thermodynamic and Kinetic Properties of Solid-Liquid Interfaces from Atomistic Simulations,* J.J. Hoyt, M. Asta, A. Karma	
9:40-10:05	*Phase Field Simulations of Dendritic Growth with Fluid Flow,* J.A. Dantzig, N. Israeli, J.-H. Jeong, N. Goldenfeld	
10:05-10:30	*Investigations of Numerical Methods for Dendritic Solidification,* S. Cummins, R. Henninger, D. Kothe, J. Quirk	
10:30-10:55	*Conduction-Limited Melting of Dendritic Mushy Zones: Experiments & Theory,* M.E. Glicksman, A. Lupulescu, M.B. Koss	

WA8 Mt. Nittany	*Polymer Mechanics (14)*	Organizers: I. J. Rao, G. Praveen Chairs: I. J. Rao, G. Praveen
9:15-9:40	*Flow Characteristics of a Multiconfigurational Viscoelastic Fluid in an Orthogonal Rheometer,* A.R. Srinivasa	
9:40-10:05	*On the Mechanism of Stress Production and Relaxation in Polymeric Melts,* R.C. Picu	
10:05-10:30	*A Thermomechanical Framework for the Glass Transition Phenomenon in Certain Polymers,* K. Kannan, I.J. Rao, K.R. Rajagopal	
10:30-10:55	*Modeling of Bimodal Networks: Incorporating Network Morphology into an Analytical Constitutive Model,* P.R. von Lockette	
10:55-11:20	*Mechanics of Shape Memory Polymers,* I.J. Rao	

Concurrent Sessions — Wednesday B, 12:35–2:40 PM

WB1 Boardrm-1	*Fractional Derivatives in Viscoelasticity (8)*	Organizers: G.A. Lesieutre, M. Enelund Chairs: G.A. Lesieutre, M. Enelund
12:35-1:00	*On the Fractional Derivative Model of Viscoelasticity,* K. Adolfsson, M. Enelund	
1:00-1:25	*Transient Response of a Viscoelastic Sandwich Beam with a Fractional Derivative Model,* A.C. Galucio, J.-F. Deu, R. Ohayon	
1:25-1:50	*On the Reduction of the Numerical Effort when Using Fractional Derivative Constitutive Equations in the Finite Element Method,* L. Gaul, A. Schmidt	
1:50-2:15	*Adaptive Discretization of Fractional Order Viscoelastic Constitutive Equations Using Sparse Time History,* K. Adolfsson, M. Enelund, S. Larsson	
2:15-2:40	*Fractional Calculus Rheological Equations of the Diffusion-Wave Type and Their Application in Mechanics of Solids,* Y.A. Rossikhin, M.V. Shitikova	

WB2 Fireside	*Ultrasonic NDE (21)*	Organizers: J.L. Rose, C. Miyasaka Chairs: J.L. Rose, C. Miyasaka
12:35-1:00	*EMAT Technique for Detection of Flank Cracks in Locomotive Wheels,* S. Jayaraman	
1:00-1:25	*Elastic Properties of Organic Thick Film by Microscopy,* J. Du	
1:25-1:50	*Analysis of Flexural Mode Tuning by Semi-analytical Finite Element Method,* T. Hayashi, J.L. Rose	
1:50-2:15	*Application of Nonlinear Acoustic Effect for Degradation Estimation of 2.25Cr-1Mo Steel Used at High Temperature,* I.K. Park, J.L. Rose	
2:15-2:40	*Damage Healing in an AS4/PEEK Composite Plate,* S. Jayaraman	

WB3 Ballrm-A	*Continuum Plasticity and Damage Mechanics (3)*	Organizers: C.J. Lissenden, G.Z. Voyiadjis Chairs: C.J. Lissenden, G.Z. Voyiadjis
12:35-1:00	*Modeling of Bone as a Hierarchical Material,* I. Jasiuk, A. Yoo	
1:00-1:25	*Strain Rate Effects on Void Growth and Coalescence,* M. Horstemeyer, M. Harbeck, P. Gullett, S. Graham	
1:25-1:50	*Sources of Heterogeneous Plastic Straining in Model Polycrystals,* T.J. Turner, M.P. Miller	
1:50-2:15	*Homogenization-Based Constitutive Models,* Y. Liu, P. Ponte Castaneda	
2:15-2:40	*The Void Size Effect on the Void Growth Rate in Ductile Materials,* B. Liu, Y. Huang, X. Qiu, K.C. Hwang, M. Li, C. Liu	

WB4 Ballrm-B	*Recent Advances in Ceramic Matrix Composites for Aeronautics and Aerospace (26) (OPEN)*	Organizer: R.M. Sullivan Chair: R.M. Sullivan
12:35-1:00	*Overview of Ceramic Matrix Composite Research at NASA for Aeronautics and Space Transportation Applications,* A.K. Misra	
1:00-1:25	*Numerical Simulation of Slurry Infiltration of Fiber-Woven Ceramic Composites,* T.A. Boarts, J. Iwan, D. Alexander, E.S. Nelson, F.I. Hurwitz	
1:25-1:50	*Effect of Environment and Material Volume on the Creep-Rupture Behavior of C/SiC,* M.J. Verrilli, A. Calomino	
1:50-2:15	*Modeling the Oxidation Kinetics of Carbon Fibers Oxidizing in a C/SiC Composite,* M.C. Halbig, J.D. Cawley, A.J. Eckel	

(more Wednesday B on next page)

Concurrent Sessions — Wednesday B, 12:35–2:40 PM

WB5 Boardrm-2	*Quantum/Atomistic/Continuum Coupling in Materials Simulation (16)*	Organizers: H.T. Johnson, W.A. Curtin Chairs: H.T. Johnson, W.A. Curtin
12:35-1:00	*Accelerated Molecular Dynamics Methods,* A.F. Voter	
1:00-1:25	*Multiscale FE/MD/QMD Method and Multimillion Atom Simulations of Nanosystems and Interfaces on Parallel Computers,* P. Vashista, R.K. Kalia, A. Nakano, M.E. Bachlechner, E. Lidorikis, S. Ogata, F. Shimojo	
1:25-1:50	*Coupled Atomistic and Discrete Dislocation Plasticity,* L. Shilkrot, W.A. Curtin, R.E. Miller	
1:50-2:15	*Multiscale Modeling of Laser Ablation of Organic Materials and Metals,* L.V. Zhigilei	
2:15-2:40	*A Continuum Description of Strain Driven Self-assembly of Quantum Dots,* V.B. Shenoy, L.B. Freund, C.V. Ciobanu, A. Ramasubramanian	

WB6 Ballrm-D	*X-ray Computed Tomography in Materials Science & Engineering (23)*	Organizers: N.L. Rupert, J.M. Wells Chairs: N.L. Rupert, J.M. Wells
12:35-1:00	*Pre- and Post Nondestructive Evaluation of Ballistically Impacted Composite Helmut Using X-ray Computed Tomographic and Thermographic Analyses,* W.H. Green, N.L. Rupert, C.G. Pergantis	
1:00-1:25	*Using Topological Rule Based Algorithms to Analyze X-Ray CT Data of Composite Microstructure,* R.S. Parnas, M. Wevers, I. Verpoest	
1:25-1:50	*Visualization of Interface Defeat Based Impact Damage in TiC Armor Ceramic,* J.M. Wells, W.H. Green, N.L. Rupert	
1:50-2:15	*Corrosion Growth Rate Study using High Resolution Computed Tomography,* C.V. Kropas-Hughes, S. Sathish, C.D. Daniels, E.L. Klosterman	
2:15-2:40	*Advanced X-ray Computed Tomography at the Army Research Laboratory: Capabilities and Applications,* W.H. Green, J.M. Wells, N.L. Rupert	

WB7 Ballrm-E	*Multiscale Modeling of Solidification (25)*	Organizers: M.F. Horstemeyer, D.B. Kothe Chairs: M.F. Horstemeyer, D.B. Kothe
12:35-1:00	*Simulating Microporosity in an Alloy,* D.R. Poirier, C. Frueh, R.G. Erdmann, P.K. Sung	
1:00-1:25	*Computational Modeling of the Vacuum Arc Remelting (VAR) Process: a Tribute to Dr. Lee A. Bertram,* R.G. Erdmann	
1:25-1:50	*Model-Based Control of Vacuum Arc Remelting,* R.L. Williamson, J.J. Beaman, D.K. Melgaard	
1:50-2:15	*Modeling of Electron Beam and Laser Welding,* M.W. Williams	
2:15-2:40	*Modeling the Spray-Rolling Process from Droplets to Spray,* S.B. Johnson, J.-P. Delplanque	

WB8 Mt. Nittany	*Polymer Mechanics (14)*	Organizers: I. J. Rao, G. Praveen Chairs: I. J. Rao, G. Praveen
12:35-1:00	*Start Up of a Nonlinear Viscoelastic Material in an Orthogonal Rheometer,* A.S. Wineman, K.R. Rajagopal	
1:00-1:25	*Constitutive Modeling of Sand Asphalt,* J.M. Krishnan, K.R. Rajagopal	

Concurrent Sessions — Wednesday C, 2:55–5:00 PM

WC1 Boardrm-1	*Fractional Derivatives in Viscoelasticity (8)*	Organizers: G.A. Lesieutre, M. Enelund Chairs: G.A. Lesieutre, M. Enelund
2:55-3:20	*Nonlinear Modeling of Elastomeric Materials,* D.S. Ramrakhyani, G. Lesieutre, E. Smith	
3:20-3:45	*Structure-borne Sound Properties of Vibration Isolators —Temperature, Frequency and Preload Dependence,* L. Kari, M. Sjoberg	
3:45-4:10	*Distributed Order Equations Arising from Physical Systems and the Existence of the Order Integral Transform Domain,* R.L. Bagley, P.J. Torvik	
4:10-4:35	*An Application of a Distributed Order Integral Equation to the Modeling of Creep,* P.J. Torvik, R.L. Bagley	

WC2 Fireside	*Ultrasonic NDE (21)*	Organizers: J.L. Rose, C. Miyasaka Chairs: J.L. Rose, C. Miyasaka
2:55-3:20	*Guided Wave Scattering in a Plate Overlap,* W.-J. Song, J.L. Rose, J.M. Galan, R. Abascal	
3:20-3:45	*Ultrasonic Inspection Using Phased Array Systems,* P.A. Meyer	
3:45-4:10	*Improved POD Methodology for Inspection Reliability Assessment using Monte Carlo Simulation,* I.K. Park, J.L. Rose	
4:10-4:35	*Ultrasonic Guided Wave Inspection Potential,* J.L. Rose	

WC3 Ballrm-A	*Continuum Plasticity and Damage Mechanics (3)*	Organizers: C.J. Lissenden, G.Z. Voyiadjis Chairs: C.J. Lissenden, G.Z. Voyiadjis
2:55-3:20	*A Restricted Slip - based Model for Variable Amplitude Multiaxial Cyclic Plasticity,* H.S. Turkmen, M.P. Miller, P.R. Dawson, J.C. Moosbrugger	
3:20-3:45	*Flow Surfaces for Fibrous Metal Matrix Composites Predicted by the Method of Cells,* L. Shen, B. Bednarcyk, S. Arnold, C. Lissenden	
3:45-4:10	*A Continuum Sensitivity Method for the Design of Deformation Processes of Materials with Ductile Damage,* S.Ganapathysubramanian, N. Zabaras	
4:10-4:35	*2D Finite Element Analysis of Angular Particulate Reinforced Aluminum,* H. Shen, C. Lissenden	
4:35-5:00	*Gradient Enhanced Finite Elements for Plasticity,* R.J. Dorgan, G.Z. Voyiadjis, E.B. Marin, D.J. Bammann	

WC4 Ballrm-B	*Recent Advances in Ceramic Matrix Composites for Aeronautics and Aerospace (26)* (CLOSED*)	Organizer: R.M. Sullivan Chair: R.M. Sullivan
2:55-3:20	*2400F CMC for Gas Turbine Application,* D. Brewer, M. Verrilli, A. Calomino	
3:20-3:45	*Properties of CMC Composites from the Second Generation RLV Design Methodology Program,* J. Koenig, J. Cuneo	
3:45-4:10	*Nonlinear Analysis of Ceramic Matrix Composites for Aerospace Applications,* B.J. Sullivan	
4:10-4:35	*Modeling of a 3-D Angle Interlock C/SiC Composite,* R.M. Sullivan, S.K. Mital, P.L.N. Murthy	
4:35-5:00	*Damping Characteristics of 3-D Reinforced C/SiC Ceramic Matrix Composite,* J.B. Min, J.M. Ting	

*ITAR restricted. Please refer to the list of Symposia by Number for instructions for access.

(more Wednesday C on next page)

Concurrent Sessions — Wednesday C, 2:55–5:00 PM

WC5 Boardrm-2	*General Topics (24)*	Organizer: C.E. Bakis Chair: TBA
2:55-3:20	*A New Experimental Setup for the Characterization of Bulk Mechanical Properties of Aerated Particulate Systems,* A.I. Abdel-Hadi, N.D. Cristescu	
3:20-3:45	*Mesoscopic Structure of Spray Formed High Strength Al-Zn-Mg-Cu Alloys,* M.M. Sharma-Judd, M.F. Amateau, T.J. Eden	

WC6 Ballrm-D	*X-ray Computed Tomography in Materials Science & Engineering (23)*	Organizers: N.L. Rupert, J.M. Wells Chairs: N.L. Rupert, J.M. Wells
2:55-3:20	*Observations of Anomalous Internal Ballistic Damage in Monolithic Ti-6Al-4V Alloy,* J.M. Wells, W.H. Green, N.L. Rupert	
3:20-3:45	*Damage Assessment in TiB2 Ceramic Armor Targets: Part I — X-ray Computer Tomography and Scanning Electron Microscope Analyses,* N.L. Rupert, J.M. Wells, W.H. Green, K.J. Doherty	
3:45-4:10	*Damage Assessment in TiB2 Ceramic Armor Targets: Part II — Radial Cracking,* N.L. Rupert, J.M. Wells, W.H. Green	

WC7 Ballrm-E	*Multiscale Modeling of Solidification (27)*	Organizers: M.F. Horstemeyer, D.B. Kothe Chairs: M.F. Horstemeyer, D.B. Kothe
2:55-3:20	*Truchas Models for Flow in Solidifying Systems: Methods and a Validation Example,* J. Sicilian, D. Kothe, M. Bussmann	
3:20-3:45	*Analysis of a Newton-Krylov Scheme for Phase Change Simulation,* J.A. Turner, B. Lally, R.C. Ferrell	
3:45-4:10	*Computational Modeling of Polymer Solidification,* M. Stan, S. Swaminarayan, K. Lam, D.B. Kothe	
4:10-4:35	*Verification and Validation of a Casting Simulation Software Tool,* K. Lam	
4:35-5:00	*Analysis of Processes Involving Heat Deposition using Constrained Optimization,* S.G. Lambrakos, R.W. Fonda, J.O. Milewski	

Plenary Abstract

Multifunctional Materials/Structures: A New Horizon in Engineering Science

Sia Nemat-Nasser*

John Dove Isaacs Chair in Natural Philosophy

Multifunctional materials and structures are systems designed and manufactured to possess one or more integrated functionality, in addition to their required mechanical and load-bearing attributes. Essentially all biological systems have integrated multifunctional capabilities. Few traditional structural systems are multifunctional. Development of multifunctional materials and hence structures requires a multidisciplinary approach that has been the hallmark of Engineering Science. Recent years have witnessed an avalanche of governmental initiative for research in multifunctional materials and structures. In this talk, I will review a class of multifunctional lightweight composites which have tuned electromagnetic (EM) signature management and sensing, self-crack-healing, thermal management, as well as being structurally strong and tough. The EM functionality is produced by integrating into the composites fabric minute amounts of conductors of optimal configuration, which leads to composites with desired electric permittivity and magnetic permeability. For example, a solid composite of this kind can be tuned to have an index of refraction of 1 over a desired frequency range, rendering the solid fully EM-transparent in that frequency range. The wire conductors are integrated into the composites fiber reinforcing braids that also include Kevlar, glass, or other desired strengthening constituents. For the matrix material, we are considering a newly developed polymer in which micro-cracks can heal, reversibly and at the molecular level, through the application of moderate heat and pressure. The conductive wires embedded in the composites can be used as resistive elements to heat the material, as sensors to detect internal damage, and as electrical conductors to tune the electromagnetic properties of the system. Multifunctional composites of this kind enhance the role of structural materials from mere load-bearing systems to lightweight structures of good thermo-mechanical attributes that also have electromagnetic and other functionalities, including self-healing. The relevant basic theory, computational simulations, experimental characterization, and processing techniques, will be briefly presented.

References

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3. D.R. Smith, D.C. Vier,W. Padilla, S.C. Nemat-Nasser, and S. Schultz. Loop-wire medium for investigating plasmons at microwave frequencies. Applied Physics Letters, 75(10):14257, 1999.

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Keynote Abstracts

Equilibrium Versus Non-Equilibrium Assembly of Nano-Structures in Solution

Jacob Israelachvili*
Professor

Atoms and molecules in solution can assemble into various types of nano-structures that can be hard (solid-like) or soft (fluid-like). Examples are small spherical micelles, hard nano-particles or quantum dots, finite or infinite cylinders or rod-like particles, or sheets. These in turn can assemble into "higher-order" structures such as ordered spheres or a continuous three-dimensional network of convoluted cylinders or sheets (e.g., nano-porous materials). Regarding the assembly processes themselves, some are thermodynamically driven and therefore occur spontaneously (spontaneous assembly). Others must be "engineered" or directed (directed assembly) by judicious inputs of energy or work that vary sequentially in space, time and temperature. Different issues arise when considering bulk and surface (film) assemblies. The talk will review the theoretical and practical aspects of different types of assemblies and assembly processes, with the aim of identifying the types of molecules and conditions that are best suited for spontaneous or directed assembly processes, and identifying outstanding issues.

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Challenges and Recent Advances in Composites for Marine Structures

Yapa D. S. Rajapakse*
Program Manager

Composite materials are being used increasingly in a wide variety of applications, including ship structures, offshore structures, and civil infrastructure. These newer applications give rise to research issues and technological challenges not encountered in aerospace applications of composites. The U.S. Office of Naval Research has established a research program in composites for marine structures, to provide the scientific basis for the effective design and use of composite materials and composite sandwich construction in affordable Naval structures with new capabilities and enhanced performance. An overview will be provided of this research program.

Examples of the use of composite materials in ship hulls and topsides in the U.S. and in Europe will be given, including monolithic composite hulls for minehunters, and advanced stealth ships built using composite sandwich construction. An advanced composite sail planned for submarines will also be discussed, as well as topside structures for the new DD(X) series of surface combatants. The unique harsh marine environment, and the effects of moisture, sea water, hydrostatic pressure, and temperature variations on marine composites, will be discussed. Affordability and quality issues will be discussed, and comparisons will be made between processing methods, including resin transfer molding (RTM) and its variations.

The presentation will also include summaries of recent research accomplishments in several areas including: effect of sea water on composite materials and sandwich structures; failure modes and failure criteria due to multi-axial loading; fatigue behavior and durability assessments; compression failure; buckling and post-buckling; impact damage; dynamic constitutive relations, and strain rate effects; dynamic failure modes; structural integrity of composite sandwich structures; dynamic behavior of composite sandwich structures; and quantitative non-destructive methods for damage assessment. Innovative experimental techniques for delineating in real-time, the evolution of dynamic failure, will be described. The advantages of the close coupling between advanced theories, innovative experiments, and computational methods in this research program will be illustrated. Future research directions will be discussed.

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Abstracts by Symposium Number

Abstracts of early-registered authors appear next, organized by symposium. The abstracts have page numbers such as "X-Y," where "X" is the symposium number and "Y" is the page number within symposium "X." The abstracts are ordered in accordance with the schedule in effect at the time this book was printed.

Active and Passive Models of Biological Tissue & Functional Engineered Tissue
(Symposium No. 1)

Organizers:
Ellen M. Arruda, University of Michigan
Karl Grosh, University of Michigan

Characterization of the Active and Passive Response of Self-Organized Cardiac Muscle Constructs

Robert G Dennis*
Assistant Professor

Ellen M Arruda*
Associate Professor

Functional cardiac muscle constructs or cardioids have been engineered in our laboratory. The tissue engineering approach used results in a cylindrical cardioid that bears a resemblance to a papillary muscle and is attached to laminin coated sutures at either end. We attach the constructs to bioreactors equipped with linear servomotors, optical force transducers and platinum electrodes for characterization of the active and passive response of these self-organized muscle tissues. Our objective is to characterize the passive response via constant true strain rate extension; several rates may be employed to examine rate dependent properties of the extra-cellular matrix. The tissue may be stimulated to contract at regular intervals via an excitation voltage supplied to the electrodes. The active response can then be explored in terms of classical tissue physiology to relate force response to excitation level, prestretch (or length) and excitation frequency. In addition we view this novel engineered material as a chemo-mechanical transducer that actively generates mechanical work. We shall also explore the ability of these cardioid constructs to dynamically change free length and stiffness as they actively generate force on a time scale of tens of milliseconds.

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Growth and Morphogenesis: A Continuum Field Theory

Krishna Garikipati* — Asst. Professor
Ellen Arruda† — Assoc. Professor
Karl Grosh‡ — Assoc. Professor
Sarah Calve§ — Graduate Research Assistant

Biological growth and morphogenesis are treated in a continuum field framework. Two classical assumptions must be relaxed to develop the theory. The first is the conservation of mass, which is replaced by mass balance when growth occurs. Mass source and flux terms are incorporated, and have implications of a fundamental nature for balance of linear and angular momentum, the dissipation inequality, and constitutive laws. The second assumption that must be abandoned is that the material microstructure remains fixed. Morphogenesis, by definition, is the contradiction of this premise. It is argued that this phenomenon requires the introduction of separate kinematic and stress-like quantities, governed by additional balance laws, and satisfying constitutive relations. This aspect of the work draws heavily from notions of configurational forces. The formulation will be presented, fundamental aspects highlighted, and some analytic examples will be solved.

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Can We Identify Vulnerable Plaques and the Location of Plaque Rupture with Numerical Methods?

G.A. Holzapfel* Th.C. Gasser* Ch.A.J. Schulze-Bauer*
Professor Researcher Researcher

Life-threatening vascular events such as myocardial infarction, stroke and sudden death are frequently due to a structural failure of a diseased vessel component. For example, it is estimated that approximately 40% to 50% of retinal and hemispheric ischemic events are related to embolic debris and thrombi originating from atherosclerotic plaque involving the carotid bifurcation. The associated culprit lesions are so-called vulnerable plaques frequently of complex morphology. The crucial clinical problem is to determine whether a plaque is vulnerable and life-threatening or remains resistant and innocuous. For unexpected catastrophic cardiac events, plaque vulnerability (and thrombogenicity) have emerged as being much more important than plaque size and stenosis severity.

Clearly, the acute event of vulnerable plaque fracture is a mechanical process. Hence, mechanical analysis may provide significant contributions regarding the identification of unstable plaques. In particular, the finite element (FE) method provides an appropriate and powerful numerical tool for investigation of the complex mechanical situation of diseased arteries. Based on reliable geometrical and mechanical data and appropriate boundary (loading) conditions, the FE method may provide insight into the tendency of fibrous cap disruption and delamination processes. In this communication we focus on delamination analyses by means of a discontinuous FE method suitable to simulate plaque fracture. The analyses are based on exact geometrical representations of embedded (strong) discontinuities using anisotropic cohesive crack models.

Based on an enhanced assumed strain field we employ a mixed finite element formulation. Thereby, an additional degree of freedom is introduced on the element level describing the displacement discontinuity. A consistent linearization of the governing equations leads to a robust and efficient FE implementation, which is required for solving large-scale FE problems of clinical relevance.

The delamination failure of a representative stenotic arterial wall is illustrated. We use high resolution MRI to obtain accurate geometrical data for the vessel wall and the highly complex plaque architecture of human arteries. The three-dimensional models of the different types of soft (biological) tissues are fitted to the experimental data.

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Nonlinear Constitutive Laws for Cochlear Outer Hair Cells

Karl Grosh* Professor | Jeffery Bischoff† Lecturer | Ellen Arruda* Professor | Niranjan Deo* Research Assistant

Outer hair cells (OHC) in the mammalian cochlea occupy a unique domain of frequency–force–displacement space in the world of electromechanical biological transduction. Under normal *in vivo* operating conditions, mammalian OHC's are electromotile up to many tens of kHz, much higher than the normal operating range of other motile tissues such as cardiac and skeletal muscle, which typically operate in the range of a few Hertz. *In vitro* measurements have shown that isolated OHCs respond to electrical stimulation at frequencies as high as 79 kHz [1]. We will show recent measurements by our group indicate that *in vivo* motility to local electrical excitation exists beyond 80 kHz. Roughly 10,000 of these nearly cylindrical 10 μm diameter by 30 μm to 70 μm long cells are present in a typical mammalian cochlea. Each cell is internally pressurized and supports a transmembrane electrical potential. This transmembrane potential is modulated by the deflection of stereocilia attached to the apical end of the OHC. The deflection arises from either fluid shear forces or mechanical loading from cells attached to the stereocilia bundle. It is this time varying change in the transmembrane potential which gives rise to *in vivo* transduction. In this paper, general nonlinear constitutive theories for the OHC material are given. These consitutive theories include electromotility and voltage dependent stiffness. A constitutive framework that encompasses both the micromechanically based laws of Iwasa [2] and the more phenomenological voltage–force dependencies of He [3] is presented. Numerical predictions of the stiffness and frequency response of the models are compared to *in vitro* experimental results.
 Work supported by grant from the NIH NIDCD (RO1-DC 04084 to KG).

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3. He D. Z. Z., Dallos P. JARO 1 (1): 64-81 AUG 2000.

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Piezoelectric-type Constitutive Relations for the Cochlear Outer Hair Cell

Alexander A. Spector*
Associate Research Professor

The outer hair cell is a receptor/effector cell located in the cochlea of the mammalian ear. This cell is a key contributor to the active amplification and sharp frequency selectivity of the ear. The outer hair cell is an elongated cylinder with a liquid core bounded by a composite membrane. The outer hair cell active properties are believed to be associated with a unique form of motility, called electromotility (Brownell et al., 1985), where the cell changes its length and radius in response to changes in its transmembrane electric potential. The major features of the behavior of this cell can be adequately represented by piezoelectric-type constitutive relationships. The electromotile dimensional changes constitute the direct piezoeffect. The deformation of the cell causes a displacement current which constitutes the converse piezoeffect. We will discuss thermodynamically consistent mechanically linear and electrically nonlinear piezoelectric constitutive relationships for the outer hair cell (Spector, 2000, 2001). At the molecular level, the electromtile behavior of the cell is related to the newly discovered motor protein, prestin (Zheng et al., 2000). We will present the results of computational modeling of electromotility of the outer hair cell on the basis of a direct representation of the molecular motors and the transmission of the motor-related active strain throughout the cell membrane (Spector et al., 2001). Since outer hair cells behaves in the cochlear as biological MEMs/piezoelectric actuators it is important to analyze the transformation of the electrical and mechanical energies and, ultimately, the effectiveness of the cell performance. We will present equations of the balance of the mechanical and electrical energies in the outer hair cell membrane. The active energy that characterizes the performance of the molecular motors has two different forms that enter the two balance equations. If the changes in the transmembrane potential are small than a linear version of the constitutive equations can be used. In this case, the two forms of the active energy coincide. One of the features of the outer hair cell is its voltage-dependent capacitance measured in a number of experiments (e.g., Kakehata and Santos-Sacchi, 1995). There are two forms of capacitance that enter the balance equations: they correspond to zero-strain and zero-resultant conditions. We will derive a relationship between these two forms of the capacitance. We will show that the zero-strain and zero-resultant capacitances provide, respectively, the lower and upper bounds of the capacitance, and the value of the effective (experimentally measured) capacitance is between these two extreme values.

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Modeling the Effects of Restructuring on the Constitutive Response of Cervical Stroma

Sebastien Febvay* Simona Socrate* Michael D. House†
Graduate Student Professor Professor

In normal pregnancies, the cervix remains firm and closed throughout gestation, while uterine smooth muscle is relaxed. Cervical stroma undergoes substantial restructuring during pregnancy where the balance of the constituent elements of the extracellular matrix (collagen, proteoglycans, elastin, water) is continually evolving. As labor begins (usually near term), the cervix softens and dilates. This maturation process occurs over the course of the last week of pregnancy and is a prerequisite for a normal course of labor and delivery. Cervical incompetence is commonly defined as a condition in which gradual, progressive, painless dilation of the cervix leads to spontaneous pregnancy loss between the second and early third trimesters of pregnancy. Cervical incompetence is often associated with an altered biochemistry of the extracellular matrix (ECM), which either mirrors the normal maturation process but occurs prematurely or, in some cases, is a congenital condition predating pregnancy. Despite the introduction of new diagnostic technologies, cervical incompetence continues to be an elusive, often misdiagnosed condition and it remains one of the leading causes of morbidity and mortality in newborn infants. Our aim is to develop a quantitative, biomechanical model that integrates cervical geometry, tissue properties and loading conditions to provide a more accurate assessment of the risk of preterm delivery and to identify appropriate management and treatment guidelines. A critical element of this study is the development of a constitutive model for the cervical tissue. The constitutive model must incorporate the ability to account for the contributions of each constituent and for the cooperative nature of the tissue response. Here we introduce a phenomenological fully three-dimensional constitutive model for the large strain, time dependent mechanical behavior of cervical tissue. The model differentiates between the roles and contributions of the collagen and proteoglycan networks under different loading conditions. In this preliminary study, we rely on in vitro mechanical tests of cervical tissue in its non-pregnant state to determine appropriate constitutive parameters. In normal pregnancies, the nature of the individual constituents evolves with cervical maturation, with substantial modifications in the degree of crosslinking in the collagen network, and the degree of tissue hydration. The proposed model framework, where the contribution of the ECM constituents are separately evaluated, will be essential in future studies to capture the evolution of constitutive behavior with cervical maturation.

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Constitutive Modelling and Material Property Determination for the Collagen Network of Articular Cartilage

V. Costanzo* Simona Socrate* Mary C. Boyce*

Graduate student Assistant Professor Professor

Articular cartilage is a complex hydrated soft tissue consisting of a small number of chondrocyte cells surrounded by an extra cellular matrix (ECM). In adults, the tissue consists primarily of a fluid component (75% by wet weight) of which a large proportion is freely exchangeable with the synovial fluid surrounding the tissue. The solid fraction of the ECM consists predominantly of a collagen network (65% by dry weight) and proteoglycans (25%), while the remaining 10% is composed of glycoproteins, lipids and chondrocytes. The collagen network and the hydrated proteoglycan (PG) macromolecules constitute an interdependent system crucial to the load bearing function of articular cartilage. The PG macromolecules consist of PG monomers bound along a filamentous backbone of hyaluronic acid. Collagen fibrils surround and intertwine among the PG macromolecules. The PG aggregates are negatively charged and interact with the free positive ions in the interstitial fluid, producing a swelling stress, which depends on the saline concentration of the fluid fraction in the tissue. In the macroscopically unloaded state, this osmotic swelling tendency is balanced against the constraining tensile forces developed in the collagen network. The ability of the collagen network to carry high internal tensile stress to balance the osmotic swelling is key to the function of cartilage. Recently, Socrate and Boyce(2001, 2002) have proposed a constitutive model for articular cartilage which independently accounts for the contributions of the key constituent material elements (the collagen network and the hydrated PG network). The proposed constitutive model follows a kinematic and constitutive framework for the large strain, time dependent deformation of elastomeric materials proposed in Bergstrom and Boyce (1998, 2000) and also successfully used to capture multiphase thermoplastic elastomeric materials in Boyce, et al (2001). A key component of the articular cartilage model is the model for the collagen network and the independent identification of material properties for this important constituent of the ECM. Following the successful work of Bischoff and Arruda (2000, 2002) in applying elastomeric network modeling strategies to the modeling of soft tissues, we present a network model for the collagenous network of articular cartilage. Utilizing literature data from osmotic stress tests, we then define a method for obtaining the needed constitutive material properties for the collagen network model. In particular, we detail how the osmotic stress test data can be reduced to provide data for the stress-stretch behavior of collagen fibrils and collagen networks when using a microstructurally-based constitutive model.

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Compliant Mechanisms
(Symposium No. 2)

Organizers:
Mary I. Frecker, The Pennsylvania State University
G.K. Ananthasuresh, University of Pennsylvania

Topology Optimization of Compliant Mechanisms and Piezoelectric Actuators for Dynamic Applications

Mary Frecker* Hima Maddisetty*

Assistant Professor Graduate Research Assistant

Compliant mechanisms are well-suited for use as coupling structures and stroke amplifiers for piezoceramic stack actuators due to their lack of joints. The compliant mechanism must be designed to have an appropriate topology and stiffness in order to work effectively with a given piezoceramic actuator for a particular application. Past efforts have been directed at developing topology optimization methods for compliant mechanisms stroke amplifiers in quasi-static applications. In the current work, a procedure is developed for designing compliant mechanisms and piezoelectric actuators in dynamic applications. The objective is to maximize the mechanical efficiency of the system under dynamic loading. The modal analysis technique is used to perform the dynamic analysis, and the design sensitivities of the objective function and the constraint equations are calculated analytically. The ground structure method is used to parameterize the design domain, where the cross-sectional areas of a network of beam elements are used as the design variables. The piezoceramic stack actuator is modeled as a single rod element, and both non-design and design cases for this element are considered. A constraint is placed on the capacitance of the piezoelectric actuator element to restrict solutions to those compatible with practical drive electronics containing switching amplifiers. A sequential linear programming algorithm has been written in Matlab to solve the optimization problem. It is found that by using a batch of randomly generated starting points, a solution that is likely to be the global optimum can be obtained. Design examples are presented to illustrate the dynamic topology optimization method and the effect of including the actuator element as a design variable in the optimization. The effects of driving frequency and external stiffness are also studied. Lastly, a comparison study is done between optimized static and dynamic compliant mechanisms and piezoelectric actuators.

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Continuum Plasticity and Damage Mechanics
(Symposium No. 3)

Organizers:
Cliff J. Lissenden, The Pennsylvania State University
George Z. Voyiadjis, Louisiana State University

A Multiscale Gradient Theory for Elastoviscoplasticity of Single Crystals

John D. Clayton* Douglas J. Bammann† David L. McDowell‡

Graduate Student Senior Research Scientist Professor

Presented first is a model for single crystal plasticity motivated by rigorous volume averaging of the kinematics of distributed discrete dislocations. We derive a three-term decomposition of the single crystalline deformation gradient. The elastic term is associated with the average applied stress and average lattice rotation in the crystalline volume element, whose size may range from a few microns (within a subgrain) to the entire single crystal. The plastic deformation gradient term is associated with the volume-averaged contribution from the history of motion of discrete dislocations. The meso-incompatibility term, here reflecting residual elastic deformation of the lattice, is absent in classical crystal plasticity theory. Following suggestions of Kroner (Int. J. Solids Structures 38, 2001), the net geometrically necessary dislocation density is obtained from volume averaging over a collection of infinitesimal Burgers circuits, while a scalar invariant of a two-point correlation function over the total discrete dislocation population expresses a total dislocation density (i.e., the sum of statistically stored dislocations (SSDs) and geometrically necessary dislocations (GNDs)).

We next develop a continuum analog of the model, wherein the displacement discontinuities associated with individual lattice defects are ignored, such that the elastic and inelastic deformation gradient terms are regarded as continuously differentiable fields. This continuum model can be considered a variant of the classical crystal elastoviscoplasticity theory of Teodosiu & Sidoroff (Int. J. Engng. Sci. 14, 1976), with three fundamental differences. Firstly, motivated by the outcome of a volume averaging procedure, we use the aforementioned enhanced decomposition for the total deformation gradient, with the meso-incompatibility term now derived as a weighted volume average of the residual microelastic deformation. This term also is shown to provide a direct description of the kinematics of grain subdivision, when relevant. The strain tensor derived from the meso-incompatibility deformation term is linked to local micro-residual elastic stress and strain fields in the crystal and hence enters the free energy expression. Secondly, strain hardening is affected through both the GND density associated with the curl of the inverse of the elastic deformation gradient and the SSD density modeled as a scalar internal variable on each slip system. Thirdly, following Le et al. (Int. J. Plasticity 14, 1998), the Eshelby energy-momentum tensor is used in the flow rule to ensure positive plastic dissipation.

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A Rational Mechanics Approach to Viscoelastic Fracture

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This paper presents a description of the thermodynamics of fracture in viscoelastic media. Utilizing the thermodynamics of the classical linear elastic fracture problem as a framework, the problem is extended to consider a viscoelastic medium. Due to the ductility encountered in viscoelastic media, the crack tip region is modeled with a damage dependent nonlinear viscoelastic cohesive zone, rather than as a single point. Both local and global thermodynamic analyses are performed for the bulk material, and the cohesive zone. These analyses result in explicit statements of the energy dissipation due to bulk viscoelasticity, cohesive zone viscoelasticity, and crack growth on both the micro- and the macroscale. These expressions are then calculated for an example problem by using a nonlinear finite element algorithm equipped with a micromechanically-based viscoelastic cohesive zone model.

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On the Coupling of Damage and Plasticity Models for Ductile Materials

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Boyd Professor Doctoral Candidate

A general concept for the analysis of a heterogeneous media that exhibits a strong coupling between viscoplasticity and damage evolution is formulated within the framework of thermodynamic laws and nonlinear continuum mechanics. The proposed formulations include thermo-viscoplasticity with anisotropic damage, a dynamic yield criterion of a von Mises type and a damage criterion, the associated flow rules, non-linear strain hardening, strain-rate hardening, temperature softening, and failure. Since the material macroscopic thermomechanical response is governed by physical mechanisms on two different length-scale levels, the macro- and mesolevel, the proposed 3-dimensional kinematical model is introduced with manifold structure accounting for discontinuous fields of dislocations interaction and microcracks and microvoids interaction. The non-local theory of plasticity and damage that incorporates microscale interstate variables and their higher order gradients at both macroscale and mesoscale levels, is used here to describe the change in the internal structure associated with these scales and in order to investigate the size effect of statistical inhomogeneity of the evolution-related viscoplasticity and damage variables. It also incorporates the thermomechanical coupling effects as well as the internal dissipative effects through the rate type covariance constitutive structure with a finite set of internal state variables. The model presented in this paper can be considered as a framework, which enables to derive various non-local and gradient viscoplasticity and damage theories by introducing simplifying assumptions.

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Experimentally Constructed Yield Surfaces for Reinforced Aluminum

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The methodology and results from an experimental study of yielding characteristics of reinforced aluminum are presented. First, newly modified yield surface determination techniques are described. Initial and subsequent yield surfaces in the axial-shear stress plane are presented for silicon carbide particulate reinforced aluminum and alumina fiber reinforced aluminum. Material hardening over various load paths is described by the evolution of the yield surface. The direction of the plastic strain increment vector is determined to assess the flow rule for these material systems.

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Modeling of Bone as a Hierarchical Material

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Bone is studied as a hierarchical composite material, consisting of several phases. The main two components are hydroxyapatite crystals that are embedded in a collagen fiber matrix. The apatite crystals are in the shape of platelets, 20x40x200 Angstroms. In trabecular bone, these crystals, placed in fibrils, are arranged in lamellar sheets (3-7 micrometer in thickness), which wind around to form randomly oriented cylindrical struts (trabeculae), about 0.1 mm in diameter and about 1 mm long. This gives trabecular bone a porous appearance at mesoscale level. Thus, bone has a complex hierarchical structure in which geometrical features occur on different length scales. In this paper we study trabecular bone as a hierarchical material. In the analysis we focus on the elastic response and damage in bone. We determine material response either analytically (using micromechanics theories) or numerically (using finite element method) at several scales, with each level being homogenized. At the lowest structural level, fibrils can be treated mathematically as inclusions with large aspect ratio, which are embedded in a collagen matrix. At the next higher up scale collagen fibers reinforced with apatite crystals form lamellae. We model it using a computational mechanics analysis of systems of hundreds (or thousands) of randomly connected collagen fibers and then employ laminate theory from mechanics of composite materials to model lamellar structure making up trabecular walls in bone. At the next scale we have a random network of struts or plates. The trabecular geometry poses modeling challenges because of its irregular structure. We account for the trabecular architecture explicitly by conducting a finite element analysis.

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Strain Rate Effects on Void Growth and Coalescence

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We analyze void growth and coalescence effects via micromechanical finite element and atomistic simulations of single and multiple voids in a various ductile metals. In our modeling effort, we start with the paradigm that voids nucleate, grow, and coelesce and we have separate continuum equations for each variable including strain rate and temperature dependence. We perform the micromechanical finite element and atomistic simulations to help determine the functional forms of the separate void growth and coalescence equations. Experiments on several ductile alloys along with the simulations will be presented showing that results are often material dependent and that the continuum equations must account for microstructural details to capture the effects.

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Sources of Heterogeneous Plastic Straining in Model Polycrystals

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Heterogeneous plastic straining is often observed in the deformation of polycrystalline materials, and manifests itself in a variety of ways depending upon the material, geometry, and applied loading. One example includes deformation induced surface roughening, or roping, seen in aluminum alloys. Surface roughening is an undesired consequence of the forming operation, as it can lead to expensive and time consuming work to remove. A more extreme example of heterogeneous plastic strain occurs at the onset of plastic instability, followed by subsequent strain localization. These phenomena are often considered detrimental to material processing as they can limit the ductility available to the deformation. Additionally, localized plastic flow can be a precursor to failure, and therefore is usually avoided as a viable deformation mode. For these reasons, the onset of plastic instability and subsequent strain localization in polycrystalline metals and alloys, are well studied phenomena.

In this paper we numerically examine the effect of geometric and material sources of strain hardening on heterogeneous plastic straining, with a particular interest in the onset of plastic instability and subsequent strain localization in model polycrystals. Geometric hardening or softening refers to the re-orientation of the crystal lattices under the applied deformation, while material hardening or softening is the increase or decrease, respectively, in the resolved shear strength on the slip systems. Both geometric and material hardening contribute to the strain hardening of crystalline materials, and both have been proposed to have an influence on the onset of plastic heterogeneity. In particular we are interested in the role of the re-orientation of the crystal lattice on localization, as textural, or geometric softening has been postulated as a mechanism for the initiation of localized plastic flow

For this work we introduce a stability criterion for polycrystalline materials based on the classical Considere condition, accounting for both material hardening of the slip systems, and geometric hardening due to the re-orientation of the crystal lattice. This criterion provides insight into the factors which are important to consider when modeling the work hardening capacity of a crystalline material. Next, we introduce a crystal plasticity based constitutive formulation, which can account for the geometric and material contributions to the stability criterion. We then employ an elasto-viscoplastic finite element formulation of the crystal plasticity formulation to examine the role of both material and geometric sources of plastic instability in model polycrystals. In particular we discuss the influence of Taylor Factor and Taylor Factor evolution on the plastic response of a polycrystalline material.

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Homogenization-Based Constitutive Models

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A fundamental problem in mechanics of materials is the computation of the macroscopic response of polycrystalline aggregates from the properties of their constituent single-crystal grains and the microstructure. In this presentation, a recently developed nonlinear homogenization method is used to compute *variational* self-consistent estimates for the effective behavior of various types of cubic and HCP viscoplastic polycrystals. In contrast with earlier estimates of the self-consistent type, such as those arising from the *incremental* and *tangent* schemes, the new estimates are found to satisfy all known bounds, even in the strongly nonlinear, rate-insensitive limit. Also, the new estimates are found to exhibit a more realistic scaling law at large grain anisotropy. Thus, for large values of the grain anisotropy M, the predictions for the overall flow stress are found to scale as M^g, where $g(0 \leq g \leq 1)$ depends on the number (less than 5) of independent slip systems that are available for plastic flow, but not on the strain-rate sensitivity. In contrast, it should be noted that the predictions of other nonlinear extensions of the self-consistent scheme are inconsistent with this scaling law. In addition, unlike the Taylor- and Sachs-type estimates, the new estimates are able to account for grain shape in a rigorous statistical sense. For all these reasons, these new *variational* self-consistent estimates are expected to be significantly more accurate than earlier estimates of the self-consistent type. Finally, it is well known that the microstructure–as characterized by the crystallographic texture and average grain shape–is found to evolve with the deformation, when the strains are large enough. The homogenization scheme allows the characterization of the evolution of the microstructure in a self-consistent fashion by making use of appropriate estimates for the average strain-rate and vorticity within the grains. The complete scheme will be described and used to model some simple deformation processes and the results will be compared with available experimental results.

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Flow Surfaces for Fibrous Metal Matrix Composites Predicted by the Method of Cells

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Just as yield surfaces are an integral part of classical plasticity theory, flow surfaces are an integral part of viscoplasticity theory. In both cases they facilitate multiaxial description of inelastic deformation and material hardening. Variants of the method of cells micromechanics model are used to predict flow surfaces for fiber-reinforced metal matrix composites. Flow surfaces based on overall and local definitions of flow are predicted in various stress planes. [0], [0/90]s, and [+45/-45]s laminated titanium and aluminum based composites are analyzed. Both the generalized method of cells and the high fidelity method of cells are used and results compared. Convergence issues for the high fidelity method of cells are addressed.

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A Restricted Slip - based Model for Variable Amplitude Multiaxial Cyclic Plasticity

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Crystal plasticity formulations based on restricted slip have shown utility in predicting elastic-plastic deformation behaviors in both large strain and small strain regimes. One of the strengths of these formulations is the availability of information fundamental to plasticity processes like crystal orientations and resulting shearing rates for all possible slip systems within an aggregate. In the present work we monitored the slip system shearing rates during cyclic loading and built relationships to strain hardening models.

We first examined uniaxial variable amplitude loading response of SS 304L at room temperature. We derived a model for cyclic hardening based on the shearing rates and accumulated shear strain within a crystal during a cycle. Pseudo-saturation levels were established for particular strain amplitudes as seen in the experimental data. We extended this model to simulations of proportional and non-proportional axial-torsional cyclic experiments. In terms of slip system activity, we observed less variation in the number of active slip systems as the phase angle was increased. At 90 degrees the number of active slip systems stayed nearly constant during a cycle. At zero degrees (proportional loading) there was much more variation in the number of active slip systems - similar to the uniaxial data. A dependence on cycle-averaged slip system activity was introduced into the hardening model to capture the differences between proportional and non-proportional responses observed in the SS 304L data.

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The Void Size Effect on the Void Growth Rate in Ductile Materials

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X. Qiu† — Graduate Student
K.C. Hwang† — Professor
M. Li‡ — Researcher
C. Liu§ — Researcher

We have extended the 1969 Rice-Tracey model of void growth to account for the void size effect based on the Taylor dislocation model, and have found that small voids tend to grow slower than large voids. For a perfectly plastic solid, the void size effect comes into play through the ratio el/R0, where l is the intrinsic material length on the order of microns, e the remote effective strain, and R0 the void size. For micron-sized voids and small remote effective strain such that el/R0 is less than or equal to 0.02, the void size influences the void growth rate only at high stress triaxialities. However, for submicron-sized voids and relatively large effective strain such that el/R0 is greater than 0.2, the void size has a significant effect on the void growth rate at all levels of stress triaxiality. We have also obtained the asymptotic solutions of void growth rate at high stress triaxialities accounting for the void size effect. For el/R0 greater than 0.2, the void growth rate scales with the square of mean stress, rather than the exponential function in the 1969 Rice-Tracey model. The void size effect in a power-law hardening solid has also been studied.

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A Continuum Sensitivity Method for the Design of Deformation Processes of Materials with Ductile Damage*

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An updated Lagrangian implicit FEM model for the analysis of large thermo-mechanically coupled hyperelastic-viscoplastic deformations of isotropic porous materials was considered in [1]. This analysis is here coupled with the continuum sensitivity framework developed in [2,3] to address important computational design problems in the deformation processing of porous materials [4]. Weak sensitivity equations are developed that are consistent with the kinematic, constitutive, contact and thermal analyses used in the solution of the direct thermomechanical problem. The present model is used to analyze a number of computational design problems in industrial metal forming processes wherein temperature and the accumulated damage play an important role in influencing the deformation mechanism, material state and shape of the deformed workpiece. In particular, preform design examples will be presented that in one- and two-stage forging processes result in a complete filling of the die cavity with desired levels of porosity and/or with other final product or process attributes. Finally, die design problems in extrusion processes will also be addressed in order to control the development of Chevron defects in the central region of the workpiece.

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2D Finite Element Analysis of Angular Particulate Reinforced Aluminum

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A generalized plane strain finite element model is used to represent a micrograph of a silicon carbide particulate-reinforced aluminum. The particles are angular, brittle, and have arbitrary size, orientation, and position. Models having particulate volume fractions of 10, 20, 40, and 60 percent are subjected to thermal loading, tension, compression, and shear loads. The constitutive law for the aluminum matrix is elastic-linear hardening. The particles are elastic until failure, which is predicted by the Rankine criterion. The particle strength is taken to be a function of particle size. Predicted overall stress-strain response as well as local stress and strain distributions are presented. The interaction between particle fracture and adjacent matrix plasticity is shown.

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Gradient Enhanced Finite Elements for Plasticity

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Scientist

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Scientist

The formulation and numerical implementation of a gradient enhanced continuum plasticity model are presented. The formulation uses a thermodynamically consistent framework as presented by Voyiadjis & Dorgan (2001) to introduce material length scales through the second order gradients of both the kinematic and isotropic hardening variables. In this formulation, the gradient dependent state variables are introduced into only the plastic potential and yield criteria to allow one to address the non-local behavior of materials and to interpret the collective behavior of defects such as dislocations. In order to give a micromechanical basis for the gradient enhanced continuum model, the evolution equations of the internal state variables derived through the gradient theory are compared to the evolution equations based on dislocation theory involving statistically stored dislocations and geometrically necessary dislocations. Based on a comparison of these evolution equations, the gradient coefficients are defined using material parameters from dislocation theory. The numerical implementation of the gradient enhanced constitutive model is made using small deformation theory and using a "low" order finite element formulation which is characterized by keeping the conventional boundary value problem (no additional boundary conditions) but the incremental tangent moduli is a function of strain and the gradients of the state variables. Details of this numerical implementation into a finite element code are presented, and boundary value problems that evaluate the effectiveness of the model by studying the mesh-dependence issue in localization problems are discussed.

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Discrete to Continuum: Mechanical Modeling Across Scales

(Symposium No. 4)

Organizers:
Gary L. Gray, The Pennsylvania State University
Francesco Costanzo, The Pennsylvania State University

An Atomistic Model-Based Continuum Analysis Incorporating the Finite Temperature Effect

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We have developed a continuum theory that is based on the interatomic potential and accounts for the finite temperature effect. It is directly linked to the interatomic potential and atomic mass, and does not introduce any fitting parameters. We have studied the thermal expansion coefficient of carbon nanotubes, and our results agree very well with the available experimental results without any parameter fitting.

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Deriving Continuum Properties from MD Simulations for Columnar Thin Films

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The optical, electromagnetic and mechanical properties of thin films (TFs) are directly correlated to their morphology at the nanoscale. This, in concert with the fact that

- new deposition techniques are enabling the growth of thin films with very complex morphologies,
- there is an increasing interest in model-based simulation (MBS) for the design of engineering structures (including nanostructures), and
- increasing computer speeds are beginning to make MBS an effective design tool capable of bridging the nanoscale with the continuum scale,

has made it increasingly important to understand how the nanostructure of a thin film impacts its properties at all length scales. The authors have developed the capability to determine the mechanical properties of thin films with amorphous nanostructure by combining molecular dynamics, *i.e.*, position of particles (*e.g.*, atoms or molecules) and their interatomic potential(s), with continuum mechanics principles. This work concerns the application of this capability to determine mechanical properties, such as stability and distributions of elastic moduli and residual stresses, to thin films grown via physical vapor deposition (PVD) under conditions in which the deposition angle of the incident species is *not* normal to the substrate. Deposition in this manner results in an amorphous thin film with a porous, columnar nanostructure, whose morphology depends primarily on the deposition angle.

In this presentation, we will focus on the exploration of the relationship between the deposition angle in PVD and the resulting mechanical properties of the film for important species such as MgF_2 and GaN. The films are created via molecular dynamics simulations using potentials available in the literature. The resulting mechanical properties are then obtained by an approach that bridges length scales from the discrete to the continuum.

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A Multiscale Continuum Mechanics Model for Predicting Damage Evolution in Inelastic Heterogeneous Media

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Professor

Damage in laminated composites is almost impossible to avoid altogether due to material mismatches and geometric features that cause unavoidable stress concentrations. Indeed, in many cases the development of damage can be so widespread as to lead to ultimate failure of structural components under both monotonic and cyclic loading conditions. The accurate prediction of this damage has in all but a few simplified scenarios eluded the scientific community, so that design tools for predicting composite life have not yet reached a state of maturity.

This paper presents a methodology for predicting the development of multiple cracks of differing types during both monotonic and cyclic loading. This methodology is based in continuum mechanics and thermodynamics for modeling this evolution of damage in elastic, viscoplastic, and viscoelastic media. The method takes advantage of the fact that damage occurs on multiple length scales in laminated composites. In particular, it is observed that microscale damage occurs ahead of delaminations (microscale), matrix cracks occur in plies (mesoscale), delaminations occurs between plies (local scale), and these interact in the structural part (global scale). Each of these scales is treated separately, and crack growth in each scale is accounted for by employing ductile fracture mechanics concepts. The results of each scale are linked to the next larger scale by utilizing damage dependent homogenization theorems, thus accurately accounting for the energy dissipation at each length scale. A computational algorithm is utilized to link the various scales and perform simulations of structural part response.

Two and three dimensional simulations of damage accumulation in laminated composite plates are presented herein to demonstrate the methodology. Examples are given for both elastic and linear viscoelastic laminated composite beams and plates subjected to both monotonic and cyclic loading. It is shown that the methodology can be utilized to predict the evolution of multiple interacting cracks.

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Connecting Discrete Atomic Model to Microcontinuum Field Theories

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Professor Professor Professor

This work aims to connect atomistic model to continuum theories. The effort includes three parts: the instantaneous mechanical variables, balance laws and constitutive relations. A physical picture of *micromorphic theory* is introduced. The fundamentals of micromorphic continuum theory, as well as its relation with various continuum theories including *Microstructure Theory*, *Micropolar Theory*, *Cosserat Theory*, and *Couple Stress Theory* are introduced. A geometric model of an atomic system is presented. The microscopic expressions of the ***instantaneous mechanical variables***, including mass, momentum, microinertia, generalized spin, body force, body couple, temperature, internal energy, stresses and heat flux, are derived in terms of atomic variables. The corresponding field quantities in continuum theory are obtained through ensemble average. The ***balance laws*** of micromorphic theory are obtained and verified from the viewpoint of molecular motion. The ***constitutive relations*** are discussed, and the approach to determine the material moduli through the molecular dynamics simulations is proposed and presented.

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Rheology and Fluid Dynamics of Micellar Solutions.

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Associate Professor Professor

Our work was motivated by an attempt to develop a rigorous mathematical model for a viscous Newtonian fluid with a large number of small worm like micells, where self-assembling soap-like molecules aggregate to form long tubular micells (worms).

Our main focus was on developing a rigorous mathematical model which (a) shows how the interaction between micellar tubes or balls affect the effective rheology of the mixture (b) provides an approximation for the effective properties of the compound.

We showed that the homogenized limit is not described by a single medium but it requires two coupled homogenized PDEs. The analysis of the homogenized problems explains the non-Newtonian overall behavior and laminarization observed in experimental studies.

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Homogenization of Polymer-Based Nanocomposites

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In this work we focus on a model polymeric material filled with spherical nanoparticles. Monte Carlo simulations are performed to determine the polymer chain conformations in the vicinity of the curved interface with the filler. The structure of the interface is determined as a function of filler size (curvature) and chain length. Models of increasing complexity are considered: an athermal system with excluded volume interactions, a system in which entropic and energetic interactions take place between polymers, and a system in which both filler-polymer and polymer-polymer energetic interactions are accounted for. The total density, chain end density, chain segment preferential orientation and chain size and shape variation with the distance from the filler are determined.

Continuum models are derived for the structures determined by atomistic simulations. The system in which polymers are well connected to the filler (strong filler-polymer interactions) is represented by a continuum composed of three phases: filler, bulk polymer matrix, and an interfacial layer with graded material properties. The system with weak interfaces (no filler-polymer interaction) is represented by a continuum model composed of two phases, filler and matrix, with a weak two-dimensional interface separating them. The parameters entering the continuum models are calibrated based on atomistic results. The continuum models are then used to homogenize the composite on larger scales. This procedure allows considering random filler distribution and clustering while accounting for atomistic detail.

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Dynamic Fracture

(Symposium No. 5)

Organizers:
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Jay R. Walton, Texas A&M University

The Velocity Gap in Single-Crystal Silicon

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Research Associate Professor Professor

Atomistic models of fracture, lattice models, predict the existence of a range of forbidden velocities at which cracks cannot propagatethe velocity gap. The velocity gap is the dynamical version of lattice trapping found by Thompson and colleagues. Molecular dynamic simulations of single-crystal silicon show velocity gap-like behavior in a more realistic setting. Here we report our results-to-date on an experimental search for the velocity gap in single-crystal silicon. Since the velocity gap is destroyed by thermal fluctuations these experiments are run at 80 K.

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Velocity Gap in Silicon

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Professor

Atomic-scale studies of fracture provide a powerful complement to traditional analysis from the continuum viewpoint. Atomic-scale methods in crystals permit calculation of fracture energies as a function of crack speed without any adjustable parameters. When the analytical methods are coupled with numerical techniques such as molecular dynamics, they lead detailed predictions for how cracks should behave in macroscopic experiments. The analytical methods also lead to some new qualitative predictions. The most important of these is the prediction of a "velocity gap;" that is, a range of velocities for which steady-state crack motion is impossible at sufficiently low temperatures. I will explain in simple physical terms the reason for the velocity gap, and talk about some of the other features of crack motion in crystals that are inaccessible from a continuum viewpoint. Finally, I will discuss the status of comparison between theory and experiment in single crystals of silicon.

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An Atomistic Study of Dynamic Brittle Fracture in Silicon

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Dynamic fracture has been modeled using a modified embedded atom method (MEAM) potential for silicon. For Mode I dynamic fracture along (111) crystallographic planes, the molecular dynamics model predicts crack speeds and fracture energies in agreement with previous experimental results [1]. In this orientation, fracture occurs almost exclusively along (111) planes for energy release rates up to 30 J/m2̂. For Mode I fracture oriented initially on (110) planes, fracture occurs by cleavage on (110) planes for a static energy release rate (J_s) less than 8 J/m2̂. For greater values of J_s, the fracture surfaces switch to alternating (111) planes, which is in agreement with previous experimental results [2]. Crack speed predictions for the (110) orientation are somewhat less than the high speeds observed experimentally.

In the atomistic simulations, the dynamically propagating cracks generate dislocations, which are primarily produced on the (111) and (110) planes. Differences in the type and quantity of dislocations produced have been observed for different orientations. Molecular dynamics has the ability to calculate the energy consumed by dislocations and other lattice defects produced during fracture and the total surface energy of the main crack, side branches and secondary cracks. The sum of the surface energy and the energy consumed by lattice defects determines the dynamic fracture toughness, J(v). The dynamic fracture toughness has been found to vary linearly with J_s. For the (111) orientation with cracks propagating in the [211] direction, J(v) asymptotically approached a value of 1/3 of J_s. The remainder of the strain energy that is released during fracture is converted into kinetic energy at the crack tip during the fracture process, which occurs atom by atom.

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Numerical and Experimental Investigations of Dynamic Interfacial Crack Growth in Composite-Homalite Bimaterials

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Dynamic crack growth along the interface of a fiber reinforced polymer composite-Homalite bimaterial subjected to impact shear loading is investigated experimentally and numerically. In the experiments, the polymer composite-Homalite specimens are impacted with a projectile causing shear dominated interfacial cracks to initiate and subsequently grow along the interface at speeds faster than the shear wave speed of Homalite. Crack growth is observed using dynamic photoelasticity in conjunction with high speed photography. The calculations are carried out for a plane stress model of the experimental configuration and are based on a cohesive surface formulation that allows crack growth, when it occurs, to emerge as a natural outcome of the deformation history. The effect of impact velocity and loading rate is explored numerically. The experiments and calculations are consistent in identifying discrete crack speed regimes within which crack growth at sustained crack speeds is possible. We present the first conclusive experimental evidence of interfacial crack speeds faster than any characteristic elastic wave speed of the more compliant material. The occurrence of this crack speed was predicted numerically and the calculations were used to design the experiments. In addition, the first experimental observation of a mother-daughter crack mechanism allowing a subsonic crack to evolve into an intersonic crack is documented. The calculations exhibit all the crack growth regimes seen in the experiments and, in addition, predict a regime with a pulse-like traction distribution along the bond line.

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Dynamic Steady-State Crack Propagation in an Anisotropic Linear Viscoelastic Body

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Considerable attention has been paid in the fracture literature to both steady-state dynamic and quasi-static fracture problems in anisotropic linear elastic material. Nearly all analyses have utilized the Stroh formalism for constructing solutions to the anisotropic linear elastic field equations, using near crack-tip asymptotic constructions to derive expressions for the dominant singular stress terms. Relatively little work has appeared treating the corresponding problem for an anisotropic linear viscoelastic body. Moreover, none of the existing solutions are rigorous; only formal constructions are presented without proof of their validity or uniqueness. Even for isotropic linear viscoelastic material, the only rigorous results in the literature assume either mode III deformations or mode I deformations in a material with constant Poisson's ratio. One of the main difficulties in the viscoelastic setting is that the approach in the elastic analyses using the elementary Stroh formalism combined with crack tip asymptotics does not work for a viscoelastic body. Presented here is a framework for carrying out a rigorous analysis of a semi-infinite generalized plane strain crack propagating in a general anisotropic linear viscoelastic body. It is evident from the analysis that no general result is possible. Rather separate cases must be considered depending upon the material's symmetry group structure and the orientation of the fracture plane relative to the material's symmetry planes and axes. The technical issues to be confronted are illustrated by presenting rigorous analyses for a general isotropic body (Poisson's ratio need not be constant) and a transversely anisotropic body. A key ingredient in the analysis is a recent result by Maurizio Romeo on the uniqueness of Rayleigh waves on a linear viscoelastic half-space.

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A Dynamically Accelerating Semi-Infinite Crack in a Linear Viscoelastic Material

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We will discuss a general solution method for a dynamically accelerating crack in a linear viscoelastic material, based on a transform method developed by Slepyan for dynamic elastic fracture problems. We treat the mode III case for crack tip speeds less than the short time shear wave speed. The analysis includes a simple explicit expression for the stress intensity factor for arbitrary time-dependent crack face traction. As examples, we apply this solution method to the Achenbach-Chao and Standard Linear Solid viscoelastic models, with a stress intensity factor fracture criterion. The method yields complete boundary values for the crack face displacement and the stress in front of the crack, so it could also potentially be applied to a cohesive zone model.

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3D Simulations for Dynamic Crack Propagation in Brittle Materials Using Rate-Dependent Cohesive Models

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Dynamic finite element analysis in conjunction with cohesive element techniques is a powerful methodology to simulate the dynamic fracture phenomenon. In the simulations, cracks are explicitly represented by cohesive elements. A cohesive law describes the opening and/or closing behaviors of the cracks. Simple and effective cohesive models have been proposed and implemented in 2D and 3D FE codes. Examples in the literature include the Smith-Ferrante law and the linear decreasing law in which the cohesive strength, σ_c, is related to a critical opening displacement, δ_c, in a way consistent with the critical energy release rate, G_c. The cohesive law is generally chosen to be rate-independent, namely, the cohesive force σ is set to be independent of the deformation-rate $d\delta/dt$ or the crack velocity v_c. For ductile materials, it is well known that due to the existence of an intrinsic time scale, rate-independent laws are successful in reproducing experimental results. However, for brittle materials, as it is computationally challenging to fully simulate the process zone at the crack tip, the effectiveness of a simpler rate-independent cohesive law is lost. It is the purpose of this paper to demonstrate the significance of a rate-dependent cohesive model.

In this paper we investigate the process of crack propagating in a pre-strained brittle PMMA strip. We begin with a brief review of experimental observations: (1) The crack velocity v_c is a function of the potential energy G stored in the strip before crack propagation; (2) The maximum crack velocity is about 60% of the Rayleigh wave speed. We proceed with numerical calculations and simulate the crack propagation behavior using a rate-independent cohesive law. It is found that the calculated crack velocity is larger than the experimental value; and that the relationship of v_c-G cannot be quantitatively obtained. To overcome this numerical limitation, we introduce a phenomenological rate-dependent cohesive law. We take the surface energy of the cohesive zone to be a function of the crack tip velocity v_c. The application of this cohesive law gives the results that are in good agreement with the experimental results. Finally, a microscopic rate-dependent cohesive law is proposed, in which the cohesive force σ is dependent on the cohesive zone opening distance, δ, and the opening rate $d\delta/dt$. The characteristics of crack propagation such as crack acceleration, limiting velocity, and crack branching, are investigated using this rate-dependent cohesive law.

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On the Use of Space-time Finite Element Method in the Solution of Dynamic Crack Propagation

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Current numerical methods used in dynamic crack propagation are of the semi-discrete type in which some numerical scheme, typically the Finite Element Method (FEM), is used to address the space component of the problem and reduce the overall problem to a system of ordinary differential equations. This approach does not lead to a transparent error estimation algorithm. In fact no results are currently available on the convergence rates of FEM solutions to dynamic fracture problems.

In this paper, a discontinuous Galerkin formulation for the solution of elasto-dynamic fracture problems is used to construct a space-time finite element approach for which a space-time error norm can be obtained. Both sharp crack problems as well problems with cohesive zones will be considered. The paper demonstrates that space-time finite element methods based on a discontinuous Galerkin formulation can be very effective in the study of dynamic fracture.

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Stress Waves and Cohesive Failure in a Finite Strip Subjected to Transient Loading

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New solutions are obtained herein for the dynamic mechanical response of a one-dimensional finite elastic strip that is cohesively bonded to a rigid substrate. Analytic solutions are obtained for a variety of cohesive zone constitutive behaviors including linear elastic, viscous, viscoelastic, and cohesive zones with evolving internal damage. Transient boundary conditions applied at the opposing end of the finite strip are both monotonic and cyclically applied in time. Results are compared to numerically obtained predictions using the explicit finite element code DYNA3D [1]. It is shown that the analytic and numerical results are essentially indistinguishable, and validate the implementation of the damage dependent cohesive zone model [2] into DYNA3D. Finally, a discussion is presented about how far-field measurements of the wave fields that interact with cohesive zones can be combined with nonlinear inverse methods [3] to either optimize the transient response of the structure or determine the cohesive zone constitutive properties.

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Experimental Verification and Validation of Virtual Internal Bond Model Parameters for Simulating Dynamic Crack Behavior

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The Virtual Internal Bond (VIB) model has been recently proposed to describe material deformation and failure under both static and dynamic loading. This is based on the incorporation of a cohesive type law in a hyperelastic framework and is capable of fracture simulation as a part of the constitutive formulation. An explicit integration scheme is better suited for the finite element implementation of the VIB model due to the difficulties arising from possible negative eigen values of the stiffness matrix for static problems. This presentation describes the explicit integration scheme implementation of the VIB model. Issues pertaining to the implementation, such as mesh size and shape dependence, loading rate dependence, crack initiation and growth characteristics, and solution time are examined. The experimental verification and validation of the VIB model has been done by calibrating the model parameters using the experimental data of Andrews and Kim (1988). The experiments involved the dynamic fragmentation of brittle materials. The simulations using the VIB model are shown to correlate well with the experimental observations.

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Dynamical Systems Methods for Advanced Diagnostics and Prognostics

(Symposium No. 6)

Organizers:
Joseph P. Cusumano, The Pennsylvania State University
David Chelidze, University of Rhode Island

Chaotic Attractor Property Analysis In Vibration-Based Structural Damage Assessment

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The primary goals of the structural health monitoring field are to provide information regarding structural performance capability, damage assessment, and even structural prognosis, all of which may potentially reduce the ownership costs associated with the maintenance and operation of the structure. Much of the research in this field has largely taken a vibration-based approach, whereby the structural dynamic response to either ambient or applied loading is analyzed for changes in certain characteristic "features" that serve as appropriate damage indicators. Many of the features proposed in the past literature have involved parameters derived from a modal analysis of the structure, e.g., resonant frequencies, mode shapes, damping, strain energy, flexibility, etc.

In this work, we present a new approach whereby the structure is excited with a chaotic input, steady-state is achieved, and various properties derived from the reconstructed output attractors are utilized as appropriate damage indicators. System characterization (including damage detection) by means of geometric invariants such as attractors is potentially a powerful generic approach which does not rely on implicit assumptions in an underlying model, e.g., linearity. The combined chaotic excitation dynamics and structural response may be thought of as the "filtering" of chaotic data: the structure acts as a "filter" through which the chaotic signal is processed so that small changes to the structure (ostensibly due to damage) will serve to alter the degree to which the signal is filtered. We show how the chaotic input may be tuned by the Kaplan-Yorke formula to provide maximum attractor sensitivity to perturbations. We develop several attractor properties such as local variance or nonlinear prediction error as candidate features and evaluate their utility (including a comparison to modal analysis techniques when possible) in various structural damage scenarios such as clamping force degradation on a beamand weld line damage on a plate.

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Detecting Measurement Noise in Chaotic Signals

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The correlation entropy and correlation dimension are measures of the predictability and structure of a chaotic system. Measurement noise, when present, creates difficulties in extracting these quantities from a time series [1]. Recently, a number of proposals for detecting and evaluating measurement noise effects have been advanced [1,2,3,4,5]. An attractive feature of Schreibers result [1,2] for Gaussian noise and Kantz and Schreibers result [1] for bounded uniform noise is their analytic expressions for contributions of noise to the correlation integral. These might aid in the search for a scaling region and they lead to a simple relationship between the embedding dimension and the inferred correlation dimension. If the results [1,2] were exact, there would be no limit on the noise level to which their expressions would apply. Here we point out that Schreibers analytic result [2] is based upon some implicit approximations. These include his setting equal to zero the projections of the embedded vectors. Using his formalism, we have derived a distinctly different one-parameter analytic approximation that results from statistical averaging. We compare, using numerical and experimental examples, exact and approximate determinations of the effects of Gaussian measurement noise.

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Vibration-based Damage Assessment Using Novel Function Statistics with Multiple Time Series

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An eight-degree-of-freedom spring-mass damper structure is simulated with a circuit experiment. The system is excited with a pre-recorded chaotic input signal and thus time series data from the output of each of the circuits in both a 'damaged' and 'undamaged' state is available with an identical input signal. This simulates output taken from a structure with multiple strain sensors, for example, with the variation of circuit parameters emulating structure damage.

In previous work by Todd, et al. [1], analysis of features from a single sensor for both a damaged and undamaged state was shown to be quite effective in assessing damage. This method used a local attractor variance ratio to detect subtle changes in the geometric features of the attractor from undamaged to damaged. It showed both robustness to noise and sensivity to levels of damage that are often an order of magnitude smaller than those detected by previously available methods.

Using multiple time series we reconstruct high-dimensional attractors for both the undamaged and damaged states. We employ a novel comparison of these attractors, the 'continuity statistic' to assess changes in the attractors between the damaged and undamaged state, and to show to what extent the damage can be localized to a particular circuit by use of this method. We also investigate use of the local attractor variance ratio in the new context of multiple time series.

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Phase Space Warping: A General Approach to Machinery Diagnosis and Prognosis

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A general dynamical systems based framework for damage tracking, diagnosis and prognosis is presented and applied experimentally. The damage evolution problem is posed as a hierarchical dynamical system with strong time scale separation [1], where the evolution of slow-time hidden damage variables causes parameter drift in a fast-time, directly observable dynamical system. The concept of Phase Space Warping (PSW) is introduced, which refers to the small distortions that occur in the fast system's vector field as a result of the underlying slowly evolving damage process. We show that a measure of PSW can be used for tracking the slow-time variables. The fast-time phase space geometry is reconstructed using delay coordinate embedding, and the degree of PSW is estimated using the short time reference model prediction error. A tracking metric is constructed using the reference model prediction error statistics for each data record.

To show the generality of the method, it is applied to two experimental systems with completely different notions of "failure." In the first, a crack in a vibrating beam propagates to failure; in the second, a potential energy is perturbed by a battery-powered electromagnet [2,3]. In both cases it is shown experimentally that the PSW tracking metric is linearly related to a scalar generalized damage variable (crack length and battery voltage, respectively). Empirical damage evolution models and recursive nonlinear filtering are used to predict remaining useful life of the experimental systems based on the tracking results. It is demonstrated that accurate estimates of remaining useful life can be made well in advance of actual failures.

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Structural Damage Prognosis Using Nonlinear Dynamics

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A nonlinear dynamical systems framework for damage prognosis is developed in this work. Simple low-order nonlinear differential equation models are shown to describe important phenomena involving the initiation and evolution of damage in prototypical test cases cited directly from the experimental mechanics literature. The two essential analytical tools for interpreting these damage models are the nonlinear local static bifurcation, which occurs whenever zero system eigen-values appear due to the change in some quasi-static operating parameter, and the notion of multiple time-scales, one which governs the overall dynamics of the system and others that govern the evolution of damage variables. The framework presented accommodates a wide variety of damage phenomena, which are observed in structural components and systems containing homogeneous (metals, polymers, etc.) and heterogeneous (metal-matrix and carbon fiber composites, thermoplastics, ceramics, etc.) materials using low order models, which are essential for on-line implementation.

The most innovative aspect of this work is its use of nonlinear bifurcations, which produce qualitative changes in damage behavior by dynamically switching between different damage "modes" that the system can experience. For example, there are three interesting damage modes to note in fatigue crack growth characteristics for homogeneous ductile materials. First, the effective applied stress must reach a certain threshold level before cracks will begin to grow out of initial flaws or existing defects in the specimen. Second, the crack growth rate is approximately a linear function (on a log-log plot) of the effective applied stress in the middle portion of the crack growth characteristic. Third, cracks experience runaway growth when a certain effective applied stress is reached. First-order nonlinear bifurcating systems can be used to transition from one damage mode to another thus generating the full set of damage modes. Even though these subsidiary damage state equations are simple, they are capable of describing the damage.

Lumped parameter analytical models of damaged mechanical systems with axial stiffness bars and transversely vibrating beams with fatigue cracks are derived and the full state responses are simulated to demonstrate how experimentally determined macro-damage component constitutive laws can be expressed within the system equations of state using multiple time scales and nonlinear bifurcations. The main emphasis is on the phenomenology of damage including fatigue cracks and loosening fasteners, the integration of the nonlinear damage model with mechanical system equations of motion, and a method by which measurable macroscopic response variables can be interpreted in near real time for prognosis using the damaged system models.

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Karhunen-Loeve Based Order Reduction of Dynamics of Flexible Structures with Application to System Modelling and Diagnosis/Prognosis of Faults

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Karhunen-Loeve (K-L) or Proper Orthogonal Decomposition modes are used to discretize and reduce the order of the dynamics of a four-bay linear truss. This is achieved by defining global K-L modal amplitudes and employing the orthogonality relations between K-L modes, inherent in the K-L decomposition. It is found that the K-L based low-order models can capture satisfactory the transient dynamics of the truss, even when only a limited number of them is used for the order reduction. A comparison between the exact and low-order dynamics in the frequency domain reveals that the low-order models capture the leading resonances of the truss. A series of experiments with a practical three-bay truss is then performed to validate the theoretical K-L decomposition. A comparison between theory and experiment indicates agreement between the dominant predicted and experimental K-L mode shapes, but less so for the higher order modes. The reasons for this discrepancy between theory and experiment are discussed. Additional applications of K-L decomposition to the identification of the dynamics and the prognosis/diagnosis of developing faults are given for a vibro-impacting beam and a rotordynamic system.

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Assessment of the Robustness of the Neuro-Fuzzy Forecasting System

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A reliable forecasting system is very useful in industry. Currently there are many time series prediction algorithms in the literature, but each has its advantages and disadvantages. According to our previous research, when a neuro-fuzzy (NF) system is properly trained, it performs better than the classical stochastic models, feed-forward neural networks, and recurrent neural networks. In this paper, the application robustness of the NF predictor is examined. After the NF system is trained using a data set from Mackey-Glass differential equation, it is implemented for different applications. First is the online health condition prognosis of gearboxes. Two test cases are utilized: a healthy gear (regular tooth wear) and a damaged gear (fatigue crack), represented by wavelet amplitude monitoring indices. Secondly, the NF predictor is applied to forecast the fault propagation trends in other research: one is a gear system with pitting damage represented by a kurtosis monitoring index, and another is a bearing response with misalignment imperfections represented by a spectral metric. Finally, the NF system is implemented for material fatigue testing for the prediction of the future states of the fatigue propagation trend of test specimens. From online tests and simulation analyses, it is found that the developed adaptive NF system is a very reliable forecasting system. It can capture the system dynamic behavior quickly and then track the system response accurately. It is also a very robust predictor, it can be applied directly to other forecasting applications represented in different scales and monitoring indices.

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Hidden Variable Tracking for Monitoring Long-Term Changes in Human Coordination

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Engineers have long been interested in how damage accumulates in mechanical systems prior to failure. Recently, methods have been developed for tracking these slowly-varying hidden processes and predicting when systems will fail [1]. These methods are based on the fact that many nonlinear dynamical systems exhibit significant "time scale separation." The system is modeled hierarchically, with a "fast-time" (observable) subsystem coupled to a "slow-time" (hidden) subsystem. By tracking, over time, appropriate state space metrics of observed time series data from these systems, the slow-time dynamics can be extracted from the fast-time dynamics [1].

Humans are often subjected to repetitive loads much like machines and, like machines, they develop repetitive stress injuries (RSI), such as carpal tunnel syndrome. However, with no firm pathophysiological model of what causes of RSI [2], it has been nearly impossible to predict who will and will not develop RSI. Furthermore, biological systems are different from mechanical systems in several critical ways. "Failure" in biological systems can occur across multiple levels, each evolving on its own time scale (cellular, tissue, organ, and system). Biological systems can heal themselves. Biological systems can also adapt their behavior to changes in their internal biology. When these changes occur slowly enough, compensatory changes in behavior may occur unconsciously. Thus, an underlying pathology may develop long before an individual is aware of it.

The methods described above are ideally suited to studying the development of RSI. Like many mechanical failures, RSI involve a substantial separation of time scales between the movements exhibited at the behavioral level and the biological injury that develops at the cellular/tissue levels. By starting from an abstract formulation of the problem in state space, these methods also avoid the need for highly detailed models of system dynamics [1], which are nearly impossible to formulate for most biological systems anyway. Finally, because they track "hidden" processes, these methods have the potential to detect how pathological changes at the cellular/tissue levels affect behavior at the observable (i.e. biomechanical) level at pre-clinical stages of disease progression (i.e. after patients begin compensating, but before they become consciously aware that they are becoming injured). If effective, such methods could lead to earlier clinical intervention, saving millions of dollars in health care costs and lost productivity. The specific challenges of implementing these methods for detecting and preventing RSI will be discussed.

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A Mathematical Model of Pulsatile Flows of Microstretch Fluids in Circular Tubes

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Pulsatile Flows of micropolar fluids with stretch whose microelements can undergo expansions and contractions besides translations and rotations in straight circular tubes are considered. The governing field equations for such flows of linear microstretch fluids turn out to be a nonlinear coupled partial differential system. Solutions are sought for this system starting with a reasonable initial approximation for microinertia and the consequent linearization of the field equations. The mathematical analysis consists in taking a finite Hankel transform of the resulting equations and solving them analytically leading to solutions in the transform space. Explicit analytical solutions for microinertia, microstretc, microrotation and velocity fields are obtained upon carrying out the inverse Hankel transforms. Successiveiteration techniques are then employed to determine higher approximation solutions in forms that are computationally suitable. These solutions have the promise of application to many practically important physical situations such as flows of polymeric fluids with deformable springy suspensions and flows of biological fluids including blood with deformable cell suspensions in small arteries.

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Probabilistic Design Analysis of Fluid Structure Interaction

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A combustor liner was computationally simulated and probabilistically evaluated in view of the several uncertainties in the aerodynamic, structural, material and thermal variables that govern the combustor liner. The interconnection between the computational fluid dynamics code and the finite element structural analysis codes was necessary to couple the thermal profiles with structural design. The stresses and their variations were evaluated at critical points on the liner. Cumulative distribution functions and sensitivity factors were computed for stress responses due to the aerodynamic, mechanical and thermal random variables. It was observed that the inlet and exit temperatures have a lot of influence on the hoop stress. For prescribed values of inlet and exit temperatures, the Reynolds number of the flow, coefficient of thermal expansion, gas emissivity and absorptivity and thermal conductivity of the material have about the same impact on the hoop stress. These results can be used to quickly identify the most critical design variables in order to optimize the design and make it cost effective.

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Advances in Crystal Growth from the Liquid Phase

Sadik Dost*
Professor

The talk focuses on the growth of single crystal semiconductors from liquid phase. Almost all electronic and optoelectronic devices need semiconductor single crystal materials. These materials are the back bone of such devices, and are produced by scientists and engineers through a process called crystal growth. Today, most semiconductors are grown from liquid phase by growth techniques known as melt/solution techniques. Among those, the solution growth techniques, Liquid Phase Electroepitaxy (LPEE) is of interest for growing thick, high quality single crystals.

In LPEE, crystalline layers from a dilute metallic solution are deposited onto a substrate of similar composition When the solution (for instance a Ga-rich Ga-In-As solution) is brought in contact with the solid (single crystal GaAs or GaInAs) substrate, growth is initiated and sustained at a constant furnace temperature by passing an electric current through the growth cell. Two mechanisms are responsible for growth: i) electromigration of In and As species towards the substrate, caused by the applied electric current, and ii) Peltier cooling at the solution-substrate interface, causing crystallization on the substrate by supercooling the solution in the vicinity of the substrate. In addition, effects such as the natural convection due to thermal and solutal gradients in the solution, the Joule heating in the source and substrate due to the passage of the electric current, the applied magnetic field, and possible finite mass transport rates at the interface may also play a significant role in the process.

LPEE has a number of advantages over other techniques. For instance, properties of semiconductors grown by LPEE show advantages over other melt growth techniques, namely, lack of detectable electron traps, low vacancy densities, low dislocation densities, and high luminescence efficiency. A very distinctive feature of the LPEE growth process is the strong stabilizing influence of the applied electric current over the composition and also on the interface. A ternary growth can begin with a binary substrate (whenever the lattice mismatch is at an acceptable level). The source can constantly supply the required materials to the solution to grow very thick crystals (so far we have grown up to 8 mm thick crystals. Due to low temperature gradients in the solution the grown crystals have less thermal stresses.

Continuum models developed for the LPEE growth process, and also the recent experimental results of the growth of InGaAs single crystals will be presented.

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On Multiple Routes to Chaos in Advection Induced by Point Vortices

Isaak Kunin* Professor

Fazle Hussain* Professor

Xiaoliang Zhou* PhD student

Chaotic advection induced by periodic motions of point vortices inside and outside of a circular domain and in the infinite plane is analyzed. Though simple, this model flow captures multiple routes to chaos and gives a good qualitative picture of advection in more complicated domains such as rectangle and ellipse. Different scenarios of chaotic advection depend on the topology of unperturbed phase portraits and type of perturbations. In addition to the typical KAM cases, we find scenarios accounting for inherent singularity of the velocity field.

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Thermo-Mechanics of Materials as a Field Theory

Gerard A. Maugin*
Professor and Chair

The complete set of equations in a well set field theory consists of the field equations (one for each field, e.g., Euler-Lagrange equations in the absence of dissipation) and the canonical or additional conservation equations. The latter involve all the fields of the theory and are related to symmetries of the whole system (e.g., via Noether's theorem in the absence of dissipation). One such equation is the energy equation for the whole system. In the mechanics of materially inhomogeneous and defective materials, it is shown that an important role is played by another such equation, the equation of canonical or pseudo-momentum. For deformable media, this is a co-vectorial equation on the material manifold itself. We shall establish the expression of that equation even in the presence of general thermodynamical processes (e.g., in heat conductors, finite-strain plasticity, irreversible theory of material growth) and prove that many, if not all, dissipative processes related to structural rearrangements of matter taking place in continua may be viewed as psuedo-inhomogeneity (equivalently, pseudo-plasticity) effects. The resulting canonical equation and its associated jump equation across a singular surface, provide the basis for the study of such theories as finite-strain anelasticity, fracture, phase transitions, a consistent theory of shock waves, as also for the design of faithful numerical schemes (those which do not produce spurious configurational forces).

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Predictability, Uncertainty, and Hyperbolicity

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Predictability of geophysical scale flows typically relies on statistical correlations of Eulerian fields. Correlation time scales determine the predictability time scale, but statistical approaches to predictability have limitations. Time series usually are short and statistical properties may be convolved with deterministic properties. Moreover, in the Eulerian framework, coherent structures are described by streamlines at fixed times. Thus in time evolving flows, typical of natural flows, there is advection across these boundaries. Finally, spatial resolution is given by wave numbers, hence, model resolution is the upper bound. Because of these shortcomings, we have been examining predictability and uncertainty in the ocean using a Lagrangian paradigm. This approach relies on calculating characteristic material curves or surfaces emanating from persistent hyperbolic regions where the fluid deformation rate dominates the flow. There are two branches to these material curves. The outflowing branch is a region of maximum stretch, the inflowing branch is characterized by maximum compression, and their intersection is a hyperbolic trajectory. In the dynamical systems literature, these branches are known respectively as the unstable and stable manifolds. These structures also form advective boundaries and channels, and delineate the boundaries of coherent structures such as mesoscale rings and eddies. Moreover, Lagrangian data are spread over space and time and generally contain information on space scales finer than model resolution. An application of the Lagrangian approach to the Gulf of Mexico is made. It is seen that blobs of fluid remain coherent, and thus predictable, until they approach hyperbolic trajectories where they undergo enormous stretching. Then an exponential increase in the uncertainty of the location of portions of the blob occurs. The loss of predictability in these cases is dramatic and sudden. We show examples where this occurs in a few hours or in several weeks. We also use the manifold geometry to devise optimal sampling strategies. Deployments of Lagrangian observations that use this strategy provide maximum spatial coverage with the least redundancy in the data. This research gives a new physical insight into predictability and uncertainty. Low predictability and high uncertainty is confined to hyperbolic regions in the flow field. Thus realistic measures of predictability and uncertainty should include this as well as the traditional statistical measures.

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Wall Effects on a Spherical Particle

Harold Ramkissoon* Rahaman Karim*
Professor Lecturer

The study of the motion of a spherical particle at the instant it passes the centre of a spherical container is important to the extent that as a model it provides some information on wall effects in the case of interaction in multipratical systems. Such a problem was investigated by Cunningham [Proc.Roy.Soc.(London) A83, 357, 1910] and then by Williams [Phil. Mag. (6th Ser) 29, 526, 1915] a few years latter. It was not until 1985 that the case of an inner fluid spherical droplet was examined by Haberman and Sayre [David W. Taylor model Bason Report No. 1143, Washington D.C, 1958]. In all these cases the no-slip condition was assumed. However, more recently the possibility of slip at the surface for a solid sphere was examined by Ramkissoon [J. Math. Sciences, 8, 59, 1997].

In this work, the question of a spheroidal container is addressed. More precisely, we examine the creeping motion of a spherical container whose shape deviates slightly from that of a sphere. An explicit expression has been obtained for the stream function associated with the flow field to first order in the small parameter characterizing the deformation. As an application we consider an oblate spherical container and determine the drag on the inner spherical particle. Wall effects are then examined and special known cases deduced.

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A Thermodynamic Framework for Describing the Flows of Anisotropic Fluids

K.R. Rajagopal*

Professor

Recently, a thermodynamic framework has been developed by Rajagopal and Srinivasa (see Journal of non-Newtonian Fluid Machanics) to describe the response of anisotropic fluids. This framework can be used to describe the flow of liquid crystals and unlike the classical theories for such materials that appeal to the notion of directors, a kinetic energy associated with the directors, body forces acting on such directors, and a balance law concerning such directors, in addition to the usual balance laws of mechanics. The framework developed by Rajagopal and Srinivasa can describe materials such as liquid crystals purely within the preview of the classical balance laws. Also, in marked contrast with director theories for liquid crystals one is not confronted with difficulties associated with prescribing conditions for the directors. In this talk, I shall describe this framework for anisotropic fluids.

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On Forces and Applications in MicroElectroMechanical Systems

Shu-Ang Zhou*

Docent

Forces, such as the gravitational force and electromagnetic forces acting between atoms and molecules, govern behaviors of our everyday things, including microelectromechanical systems (MEMS) that are being developed rapidly in recent years due to the maturing of their fabrication processes and their wide possible applications in automobiles, biomedicine, optical, and wireless (radio) communication systems. Without an understanding of dominating forces in MEMS, many phenomena, such as kinetics, dynamics, stiction, friction, adhesion, wear etc. in MEMS, cannot however be explained scientifically, and consequently, the great potential of MEMS technology could neither be explored effectively, nor be utilized optimally. This paper is therefore an effort of investigating the basic forces of importance in microelectromechanical systems, their origin, effective range of action, proper classification, and mathematical formulations.

Studies have shown that although most of mechanical components in MEMS have a size scaled at micrometers, they may approach to each other during their mechanical motions in a distance of nanometers, or have even direct contact during switching functions. Operating at surfaces, across interfaces, and between micro-mechanical components, intermolecular and surface forces may therefore play an important role, which could determine ultimately our success or failure in the design, fabrication, and applications of microelectromechanical systems. It is also shown that interactions between macroscopic bodies in MEMS structures can be effectively of much longer range than those between molecules even though the same type of force may be operating in each case, depending on the shape and size of the macroscopic bodies. Because of the extremely small size of micro-mechanical components in MEMS, the size-effect on their interaction forces can be significant and will therefore be studied and formulated in the paper. Furthermore, interaction forces are shown to be dependent on interacting media, their physical properties. A comparison of some major operating forces in MEMS is made quantitatively with respect to the interaction range of the media. Possible applications are also explored for some microelectromechanical systems in which a variety of forces may play significant roles.

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Application of Nonlocal Continuum Models to Nanotechnology

John Peddieson*
Professor

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Professor and Dept. Head Emeritus

The length scales associated with nanotechnology are often sufficiently small to call the applicability of classical continuum models into question. Atomic and molecular models, while certainly conceptually valid for small length scales, are difficult to formulate accurately and are almost always computationally intensive. Nonlocal continuum models represent attempts to extend the continuum approach to smaller length scales while retaining most of its many advantages.

A problem of current interest is the development of small actuators in the form of cantilever beams exhibiting elastic response. In the classical (local) elastic model the stress state at a given point is regarded as being determined uniquely by the strain state at that same point. In the nonlocal model, on the other hand, the stress state at a given point is regarded as being determined by the strain states of all points in a finite neighborhood of the given point. This recognizes the finite range of interatomic and intermolecular forces. While the constitutive equation of classical elasticity is an algebraic relationship between the stress and strain tensors, that of nonlocal elasticity involves spatial integrals which represent weighted averages of the contributions of the strain tensors of all points in the neighborhood of the given point to the stress tensor at the given point. Under certain conditions these integral constitutive equations can be converted to equivalent differential constitutive equations.

In the present work, the Bernoulli/Euler beam model is extended to include nonlocal elastic material response. Issues related to boundary conditions are discussed and several closed form solutions are presented. An attempt is then made, based on these solutions, to identify the parametric range for which nonlocal effects will be important in practical actuator applications.

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Length-Scale in Plasticity

Sia Nemat-Nasser*

Professor and Director

Plastic deformation of a broad class of metals occurs by the motion of dislocations. The structure of dislocations, their density and distribution, as well as their interaction with each other and with the solute atoms lie at the foundation of crystal plasticity. The resistance that these events naturally impose on the dislocations defines the flow stress of the material at the continuum scale. Based on the results of systematic experiments on numerous commercially pure metals, the rate- and temperature-dependence of the flow-stress has been modeled by the author. This modeling naturally involves length-scales that characterize the underpinning dislocation activities. It will be shown that the introduction of the density of the dislocations and its evolution into the constitutive relations is sufficient to account for essentially all existing experimental results. In addition, the phenomenon of dynamic strain-aging that involves the interaction between dislocations and solute atoms is modeled, and will be illustrated.

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On Extracting Physical Information from Mathematical Models of Chaotic and Complex Systems

Isaak Kunin*

Professor

During the last three decades the interest to chaotic and complex systems was growing with exponential rate and with major emphasis on mathematical aspects of these phenomena. At the same time the crucial problem of extracting adequate physical information from these systems practically has not been addressed. One of the possible explanations: the problem is highly multistructural. It requires joint efforts of specialists in mathematics, mechanics, physics, engineering, etc. Recently an international group of researchers in these fields has decided to combine their efforts in attacking this important and highly challenging problem from different directions.

One of approaches is based on analogy with quantum mechanics which stays on two legs: states and observables. To introduce them in this contex it is convenient to distinguish mathematical (MD) and physical (PhD) dynamical systems.

MD system is a classical system (continuous or discrete, regular or chaotic) that defines states

PhD systems have the following typical components:

Physical realization of a chosen MD system (e.g. Lorenz system has a dozen different realizations)

Induced structures: Hamiltonian, dissipation-pumping, characteristic micro- and macroscales

Space-time quantization (group deformation)

Observables respecting Kolmogorov Complexity theory (that rejects infinite computational algorithms and precision)

All physical information is on the shoulders of observables

Gauge invariance leads to physical degrees of freedom

Optimal gauge results in order in chaos and new definitions: K-order, Kaos

Numerical algorithm with the corresponding parameters is an intrinsic part of the PhD system

Notice: this approach is a step towards coexistence for pure mathematics and reality

The presentation reviews approaches to the problem and gives examples of their applications.

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Surface Cracking of Graded Materials Due to Sliding Contact

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Graded materials also known as functionally graded materials (FGMs) are generally two-phase composites with continuously varying volume fractions. Used as coatings and interfacial zones they tend to reduce stresses resulting from the material property mismatch, increase the bonding strength, improve the surface properties, and provide protection against adverse thermal and chemical environments. Thus, the concept of grading the thermomechanical properties of materials provides material scientists and engineers with an important tool to design new materials for specific applications. To take full advantage of this new tool research is needed not only for developing efficient processing and characterization techniques but also for carrying out basic mechanics studies relating to the safety and durability of FGM components. Many of the present and potential applications of FGMs involve contact problems. These are mostly the load transfer problems between two deformable solids, generally in the presence of friction. From the viewpoint of failure mechanics an important aspect of sliding contact problems is surface cracking which is caused by friction forces.

With the application to fretting fatigue in mind, the main objective of this study is to investigate the problem of contact mechanics in graded elastic solids. The physical problem is the initiation and propagation of surface cracks under repeated loading. Examination of crack initiation requires the determination of the in-plane stress in addition to contact stresses on the surface, whereas the crack propagation requires the evaluation of the stress intensity factors at the crack tip. It is assumed that the contacting solids are in relative motion and contact stresses are related thorough Coulomb friction. The coupled crack/contact problem for a graded half-plane with a surface crack and loaded by a moving rigid stamp of an arbitrary profile is formulated. The singular behavior of the solution and fundamental functions of the problem are obtained by using the function-theoretic method. The new results regarding the singularity of the coupled crack/contact problems are independently verified by using the standard Mellin transform. The problem is solved numerically and some sample results are presented to show the influence of the friction and material inhomogeneity on the stress intensity factors.

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Constitutive Relations of Micromorphic Thermoplasticity

James D. Lee* Youping Chen*
Professor Researcher

This work is concerned with a micromorphic theory of thermo-visco-elastic-plastic materials. Emphasis is on the development of the constitutive relations of microcontinuum theory with full utilization of thermodynamics.

The nonlinear theory of micromorphic elasticity was first published by Eringen and Suhubi in 1964. Since then Eringen has developed numerous constitutive theories for various types of materials. Micromorphic theory is a continuum field theory for continua that posses microstructures. A micro-continuum is defined as a continuous collection of deformable point particles which may be interpreted as polyatomic molecules, crystallites of a polycrystal, or grains of a granular material. The macro-motion defines the movement of the centroid of a point particle and the micro-motion accounts for the inner motions of the material points within the point particle.

The generalized Lagrangian strains and their corresponding higher order deformation rate tensors obtained recursively are shown to be objective. In the development of thermoplasticity, the generalized Lagrangian strains, strain rates, temperature, temperature gradient and internal state variables are taken as independent constitutive variables. The dependent constitutive variables (Helmholtz free energy, entropy, generalized Cauchy stresses, and heat flux), the yield function, and the evolution functions of the internal state variables are assumed to be functions of the independent constitutive variables as a the axiom of equipresence suggests. In this work, the Clausius-Duhem inequality is adopted as the mathematical description of the second law of thermodynamics. During the entire process of formulating the theory of micromorphic thermoplasticity the Clausius-Duhem inequality serves as a binding guidance. Various special theories can be deduced based on material symmetrics and/or conventionally adopted assumptions. The applications to plastic problems in microsystems, shear band, and dynamic crack propagation are discussed.

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The Contributions of Microrotation of Lubricant Molecules in a Journal Bearing

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Professor

Characteristics of a journal bearing were computed for thin film lubrication accounting for microrotation of the lubricant molecules using the micropolar fluid theory. Both the half-Sommerfeld and Reynolds boundary conditions were considered. The results based on both these boundary conditions show noticeable differences in pressure distribution and load profiles. The pressure distribution for the Reynolds solution is more realistic, especially at the journal outlet point. In comparison with Newtonian fluids, the micropolar liquid lubrication can produce the load positively or negatively, depending upon the characteristics of the interacting surfaces and the lubricant. Larger loads are realized when the fluid is retarded at the surfaces, whereas less retarded fluids result in smaller loads. The effect was amplified by the magnitude of the coupling number and material length.

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Discrete Systems of Controlled Pendulum Type

Boris Yamrom* Isaak Kunin† Ralf Metcalfe‡ German Chernykh§

Professor Professor Professor PhD Student

A challenging class of controlled pendulum (CP) type systems has been introduced in one of the papers presented at this Symposium, wherein examples treated by standard floating-point methods were given, This presentation applies recently developed discrete methods to the same CP type systems with two goals: a) Comparing results obtained from two methods; b) Extracting additional information that in principle cannot be obtained using floating point methods, such as discrete cycles, transients leading to such cycles, etc.

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Lorenz-Type Controlled Pendulum

Isaak Kunin* Boris Kunin†
Professor Professor

It is known that the famous Lorenz system admits several physical realizations. One of them is mechanical: Duffing system with a state feedback control, or controlled Duffing (for short CD). It is also known that the Duffing system approximates oscillations of a pendulum with small amplitude. As a consequence, a circle configuration space for the pendulum is substituted by the straight line. This motivates introducing a new class of controlled pendulum (CP) systems that may also be interpreted as Pendulum-Lorenz systems. These systems contain the Lorenz system as an approximation and may have a wide range of potential applications, in particular to engineering problems. Comparison of CD and CP shows instructive analogies and differences of these systems for both chaotic and regular regimes. This may be considered as a step towards introducing a more general family of Lorenz-type systems.

The presentation gives a review of CP systems and examples of applications.

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Kolmogorov Complexity and Chaotic Phenomenon

Vladik Kreinovich*
Professor

Isaak Kunin†
Professor

Born about three decades ago, Kolmogorov Complexity Theory (KC) led to important discoveries that, in particular, give a new understanding of the fundamental problem: interrelations between classical continuum mathematics and reality (physics, biology, engineering sciences, ...). Some statements of KC in simplifying form:

- KC rejects the assumption of infinite computational and observational algorithms and precision
- Infinite sequences having maximum complexity are incalculable
- Roughly speaking, it is important to distinguish "human" and "inhuman" numbers (like $10^{10^{10}}$ which is much bigger than the number of particles in the Universe).
- Only finite "human" algorithms are adequate to describe reality

Notice: it is shown that almost all chaotic orbits have maximum complexity $\Rightarrow$ they are incalculable. The goal of this presentation is to show that ideas and methods of KC may play a crucial role for extracting physical information from chaotic systems. Vice versa, this interaction will stimulate further development of KC in physical directions.

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A New Geometrical Approach to Chaos

Serge Preston* Isaak Kunin† Juri Gliklikh‡

Professor Professor Professor

A new geometrical approach to the description of chaotic phenomena in dynamical systems is suggested. It is shown that a certain 1-1 tensor field generated by a chaotic dynamical system may be interpreted as a deformation gradient in mechanical terms or as an affine connection in geometrical terms. The corresponding curvature tensor gives a new measure of chaotic behavior. This tensor may be considered as a far reaching generalization of the well-known Lyapunov exponents.

Numerical algorithm for the calculation of this connection and the corresponding curvature is suggested. Examples are considered, including popular Lorenz and Rssler dynamical systems.

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Model Reduction of Large Space Structures Using Approximate Component Cost Analysis

Karolos Grigoriadis* Isaak Kunin*
Assoc. Professor Professor

System analysis, simulation and control design objectives often dictate the need to approximate high-order dynamical systems by lower-order ones. A number of model reduction methodologies, such as balanced truncation , Hankel-norm approximation , and optimal L2 and H-Infinity methods, have been developed in the past two decades to address this objective. In particular, model reduction plays an indispensable role in the analysis and control of flexible space structures since these systems are by nature distributed parameter, and discretization methods result in high-order dynamic models.

A state-space methodology that is particularly suitable for the model reduction of multi-body flexible structural systems is component cost analysis (CCA). CCA associates a component output cost with each system state or component. Then, the system components are ranked according to their cost contribution and reduced-order models are obtained by deleting (truncating) the states with the smallest cost. CCA has been applied successfully to obtain reduced-order models of space systems and flexible structures.

In CCA, the computation of the component costs requires the solution of a Lyapunov equation of order equal to the order of the full-order system. However, in many engineering applications, multiple model reductions of very large scale systems are required for simulation and control design purposes. For example, finite element modeling of large multi-body space structures, such as the International Space Station (ISS), could result in systems with several hundreds or thousands of states. Solution of Lyapunov equations of this order is difficult or prohibitive to obtain due to excessive computational time and storage requirements.

In this work, the use of Krylov-subspace iterative methods are proposed to obtain low-rank approximate solutions of large Lyapunov equations for approximate CCA model reduction of very large scale systems. Cost-equivalent and cost decoupled realization using the approximate Krylov-subspace solutions are developed. The methods are applied to obtain reduced-order models for several ISS assembly stages and extensive comparisons with the standard methods are provided. It is shown that the proposed approximate CCA methods are computationally efficient and produce close approximations of the exact CCA solutions.

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Size Dependent Material Behavior at the Micron and Sub-micron Scales

Yonggang Young Huang*
Professor

The conventional continuum theories are successful for macro-scale (greater than 100 microns) applications, but fail to predict the material behavior observed at the meso-scale (0.1 to 10 microns) such as the depth-dependent indentation hardness. Because of the technical importance at the mesoscale, we propose a meso-scale continuum theory, namely mechanism-based strain gradient (MSG) plasticity, based on dislocation mechanics at the micro-scale (less than 0.1 micron). This theory bridges the gap between continuum plasticity and dislocation mechanics and is intended for applications to materials and structures whose dimension controlling plastic deformation falls roughly within a range from 0.1 to 10 microns (e.g., MEMS, thin film, micro-electronics and optoelectronic devices, composite materials). In order to validate this new continuum theory, we compare with meso-scale experiments such as micro-indentation hardness tests, micro-twisting of thin wires, micro-bending of thin beams, particle-reinforcing composites, and MEMS. The development of MSG plasticity theory allows us to investigate a range of phenomena that cannot be well addressed by conventional continuum theories.

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Fractional Derivatives in Viscoelasticity
(Symposium No. 8)

Organizers:
George A. Lesieutre, The Pennsylvania State University
Mikael Enelund, Chalmers University of Technology

On the Fractional Derivative Model of Viscoelasticity

Klas Adolfsson* Mikael Enelund*
PhD Student Assoc. Prof.

By introducing fractional order derivative or integral operators instead of integer order operators in the viscoelastic constitutive equations it is possible to describe the observed material behavior of many viscoelastic materials using only a few model parameters. The resulting models are here denoted fractional order viscoelastic models and can be seen as generalizations of the classical standard viscoelastic model. In particular, the fractional models can describe the weak frequency dependence of the damping properties and the stress relaxation or the creep over long time intervals.

We use the concept of internal variables of strain type in the viscoelastic model. The internal variables then model the dissipation. The evolution equations for the internal variables involve fractional order operators either derivatives of orders $\alpha \in (0, 1)$ or integrals of orders $\beta \in (0, 1)$. If fractional integral operators are used, two operators enter in each evolution equation whereas only one enters if fractional derivative operators are used. However, from a numerical point of view fractional integral operators are advantageous as their kernel functions are less singular and therefore easier to handle. We show that the internal variables can be expressed in terms of the strain as convolution integrals with kernels of Mittag-Leffler function type. The parameters of the model are physically interpreted from viscoelastic functions like the stress relaxation function and the corresponding spectrum. A motivation for using fractional derivatives in viscoelasticity is that a whole spectrum of damping mechanisms can be included in a single internal variable. By a suitable choice of material parameters for the classical viscoelastic model (based on integer order derivatives) we observe both numerically and analytically that the classical model with a large number of internal variables (each representing a specific damping mechanism) converges to the fractional model with a single internal variable.

Finally, we discuss the thermodynamic background of the fractional viscoelastic model. By counter examples we show that the dissipation inequality in its spatially and temporally strong form is not generally satisfied while its temporally weak form is generally satisfied. This means that the dissipation power is not necessarily non-negative whereas the dissipation work is non-negative.

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Transient Response of a Viscoelastic Sandwich Beam with a Fractional Derivative Model

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J.-F. Deü* — Assistant Professor
R. Ohayon* — Professor

A finite element formulation for a sandwich cantilevered beam with a viscoelastic core is developed to simulate transient response originated from time impulses, using a fractional derivative model. Such a structure has numerous applications in aerospace industry, notably for active/passive vibration control using viscoelastic layers and piezoelectric patches [1]. One of the main advantages of employing a fractional derivative formulation is the possibility of representing the material damping over a wide broad of frequency using a relatively small number of parameters (if compared to classical models, as ADF and GHM, for example). In this study, the four-parameters fractional derivative introduced by Bagley and Torvik [2] is employed to describe the damping behavior of the viscoelastic material. In the finite element implementation of the sandwich beam, a direct time integration method is proposed, based on previous investigations [3]. This solution strategy consists of shifting the frequency dependence of the stiffness matrix to the right-hand member of the governing equation. This kind of approach is useful for treating non-linear problems, which constitutes the next step of this research. The Grunwald's formulation for fractional derivatives is applied to the stress-strain constitutive equation and an adaptation of the Newmark's method is used to solve the governing equations. When such a formulation is employed, some difficulties arise when determining the numbers of terms to be retained in the time stress history and the influence of the time step on the damping present in the transient response. Consequently, it is necessary to develop some criteria for truncation (fading memory phenomena) and time discretization. Moreover, the master curves for the viscoelastic material are presented, showing the agreement between the fractional model, a classical model and the measured data. The small number of parameters needed for the fractional model is emphasized as well as the good smoothness of the master curves. In this way, a strategy to carry out the identification of these parameters is developed.

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Adaptive Discretization of Fractional Order Viscoelastic Constitutive Equations Using Sparse Time History

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By using fractional order derivative operators or fractional order integral operators in the constitutive theory of viscoelasticity it is possible to capture the behavior of many viscoelastic materials using only a few model parameters. The drawback of these models is that when numerically integrating the constitutive response the whole previous strain history must be saved and included in each time step. The most commonly used algorithms for this integration are based on the Lubich convolution quadrature for fractional order operators which is, in its first order form, equivalent to a truncation of the Grunwald definition of fractional differentiation and integration. The Lubich convolution quadrature requires uniformly distributed time steps. This is a cumbersome restriction because it is not possible to use adaptivity and goal-oriented error estimates. From an engineering viewpoint it is important to assess the quality of the numerical algorithm with respect to its capability to predict responses with high accuracy. This means that goal-oriented error estimates should be used. Here we develop an adaptive algorithm with a priori and a posteriori error estimations for the integration of fractional order equations. We use a viscoelastic formulation that is based on the concept of internal variables. The evolution equations for the internal variables involve fractional order operators and may be identified as Volterra integral equations with singular kernels. For the numerical integration of these equations we adopt the discontinuous Galerkin method with piecewise constant basis functions. This method is in particular well suited for singular kernels in that the convolution integrals enter in the form of averages instead of point values. The method can handle variable time steps which enables us to use adaptivity. An a posteriori error estimation based on the solution to an adjoint problem of the evolution equations is the basis for the adaptive strategy. To overcome the problem with the growing amount of data that has to be stored and used in each time step we introduce sparse quadrature. Sparsely distributed time steps are used in the distant part of the history while small steps are used in the most recent part. The idea is to break up the convolution structure by using piecewise linear interpolants between the large steps in the distant part of the history. The precision and effectiveness of the present algorithm are very good with respect to the analytical solution of the stress response to a unit strain.

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Nonlinear Modeling of Elastomeric Materials

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A new one-dimensional model of the dynamic behavior of elastomeric materials is developed based on a previously existing model. The older model consisted of nonlinear multiple Anelastic Displacement Fields in parallel with discrete friction elements. The motivation for the development of the new model is reduction of the number of parameters used to capture material behavior relative to that required in the older model.

A new element, called a continuously yielding element, is developed, which conceptually represents an infinite number of friction elements in parallel. This element is used to replace the entire collection of discrete friction elements used in the older model. In addition, a linear fractional derivative Anelastic Displacement Field model is used to replace the linear multiple Anelastic Displacement Field elements used in the older model. Finally, nonlinearity is introduced into the fractional derivative Anelastic Displacement Field element, in an attempt to capture observed amplitude dependence at higher amplitudes.

Grunwald's definition of the fractional derivative is used for time integration of this model. The history required to calculate the present value of the fractional derivative is truncated to reduce computational effort. The resulting error is reduced using weighting functions to modify the truncated history. Two kinds of weighting functions were used for this purpose. One used a constant value to multiply the truncated history. The other used exponential weighting in which more recent values were weighted more than those further in the past. Non-linearity is introduced by making these weighting functions amplitude dependent, so that the weighting function behaves as a constant weighting function at lower amplitudes and as an exponential weighting function at higher amplitudes.

The parameters of the new model are obtained by adjusting those of the individual parts of the new model, in order to match the behavior of the corresponding parts of the older model. The continuously yielding element has smoother behavior when compared to that of the discrete friction elements, and uses two parameters instead of six. The linear fractional derivative element captures the variation of the linearized modulus with frequency very well, better than the multiple linear Anelastic Displacement Field elements of the older model do. When nonlinearity is introduced in the fractional derivative element, its behavior does not quite match that of the nonlinear multiple Anelastic Displacement Field elements.

The different parts of the model are combined and the two models are compared. The new model shows similar behavior in the frequency and amplitude range of interest, while the total number of parameters is reduced to eight from sixteen.

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Structure-borne Sound Properties of Vibration Isolators —Temperature, Frequency and Preload Dependence

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A nonlinear, frequency, temperature and preload dependent dynamic stiffness model of a natural rubber vibration isolator is presented in the audible frequency range; covering 20 to 20 000 Hz, −50 to +50 ℃ and 0 to 20 % precompression.

A nearly incompressible, thermo-rheologically simple material model is adopted, being elastic in dilatation while displaying viscoelasticity in deviation; the latter exhibiting a time–strain separable relaxation tensor with a single Mittag–Leffler function embodying its time dependence. This fractional derivative based function, having a continuous distribution of relaxation time, is shown to successfully fit the results of dynamic mechanical thermal analyzer measurements throughout the whole audible frequency range while employing the method of reduced variables using a William–Landel–Ferry equation for the temperature–frequency shifts. An extended neo-Hookean free energy function, being directly proportional to the temperature and density, is applied for the finite deformation response. The weak formulations corresponding to the stiffness problem are solved by an updated Lagrangian nonlinear finite element procedure.

The stiffness is found to depend strongly on audible frequencies—resulting in acoustic resonance phenomena such as stiffness peaks and troughs, and on preload—resulting in a low-frequency stiffness increase and peak and trough shifts to higher frequencies, and, finally, on temperature.

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Distributed Order Equations Arising from Physical Systems and the Existence of the Order Integral Transform Domain

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Professor Emeritus

Caputo's application of the fractional calculus to the description of mechanical response of viscoelastic materials over 30 years ago spawned a renewed interest in the application of this branch of calculus to systems of engineering interest. Contained in his seminal work (ref. 1) was the suggestion that equations containing operators, having differential order that varied continuously over a finite range, might arise in the description of physical systems. More recent work (ref. 2), applying the fractional calculus to viscoelasticity, suggests that the order of differentiation in the stress strain relationship may be temperature dependent. Consequently, the mathematical volume averaging, either for finite element or homogenization formulations of the mechanical properties of a viscoelastic medium with a spatially varying temperature field, will result in a differential equation containing a distribution of orders of differentiation. The resulting distributed order differential equation can be recast as distributed order integral equation. The resulting integral equation contains a weighted spectrum of Riemann-Liouville fractional order intgrals of the solution function. The solution of the integral equation contains a weighted spectrum of fractional order integrals (ref. 3) as well. In both the integral equation and its solution the order of integration is denoted with an order variable called the order parameter. In the process of developing a solution technique for distributed order integral equations, we discovered an integral transform domain, based exclusively on the order parameter, that has some utility in solving distributed order integral equations (ref. 4). Both forward and inverse integral transforms will be shown, as well as their relationship to Laplace transforms.

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An Application of a Distributed Order Integral Equation to the Modeling of Creep

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Material models incorporating fractional derivatives of the dependent variables (stress and strain) with respect to time have received considerable attention over the past two decades, particularly in regard to the modeling the response of polymeric materials to sinusoidal loads. When the fractional derivative is employed, significantly fewer material parameters are required to match the observed response over many decades of frequency. This led us consider (Ref. 1) allowing the order of differentiation of the fractional derivatives to take on continuous values of an order parameter, treated as the independent variable in a new order domain. The proposed constitutive equation is then formed by integrating over the allowed range of the order parameter.

The resulting distributed order differential equation is recast as a istributed order integral equation, with integral over the distributed order of the Riemann-Liouville fractional order integral. We have also given (Ref. 2) a method for solving such equations. In obtaining a solution, each of the time dependent quantities is represented as a generalized Taylor series, for which the integration spectrum is a function of the integration order in the original equation. These spectra then provide representations of each such function in an order domain, the use of which facilitates obtaining a solution.

In the present paper, we first summarize that method of solution, and then apply it to such distributed order integral equations as might arise in the modeling of creep. The dependent variable is taken to be strain, and the right hand side is developed from a step input in stress. Several different distributions of the differentiation order are considered. The time dependent strains resulting from such constitutive equations are compared with the creep response resulting from an assumption of linear viscosity (integer derivatives) and to the response for constitutive relationships incorporating one or more fractional derivatives of discrete order.

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Growth in Biological Tissues

(Symposium No. 9)

Organizers:
I. Joga Rao, New Jersey Institute of Technology
Grama Praveen, General Electric Corporate R&D

Heterogeneity in Myocardial Structure Correlates Well with Heterogeneity in the Strain Field

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Thermo-Mechanical Degradation of Rubber:Mechanical Consequences and Implications for Soft Tissue Modeling

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Professor Student

Rubber and soft biological tissues are usually modeled as nonlinear elastic materials. Inherent in nonlinear elasticity is the assumption that stress is produced by the distortion of a network of crosslinked macromolecules, and that the underlying structure of this network does not change. Recently, models for rubber have been studied that account for changes in microstructure occurring at high temperatures. The modeling concepts and microstructural events may be applicable to the study of soft biological tissue undergoing changes.

The changes in a rubber at a sufficiently high temperature result from time dependent scission of its macromolecular network junctions. The affected molecules recoil and re-crosslink to form new networks that are stress free in new reference configurations. If this process occurs while the rubber is deforming, it becomes a time dependent mixture of molecular networks with different reference states. A constitutive theory is presented which accounts for this process.

This constitutive theory is used to study a pressurized spherical rubber membrane undergoing the scission-cross linking process. Because of changes in the material properties, there is a finite time when the sphere diameter can begin to rapidly expand and even increase at an infinite rate, i. e. blow out. This depends on the elastic properties of the molecular networks, the rate of formation of new networks, and the history of the increase in the membrane diameter. Numerical results are presented for the case when the networks act as Mooney-Rivlin materials.

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A Constrained Mixture Model for Biological Growth and Remodeling

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J. D. Humphrey† — Professor
K. R. Rajagopal‡ — Professor

A number of recent papers have demonstrated the importance of mechanotransduction on changes in structure and function, including the growth and remodeling process. Examples of this phenomenon include vascular adaptation to hypertension, microgravity, balloon angioplasty and compliance mismatch due to synthetic grafts. These transformations are due to stress-induced changes in cellular activity including rates of mitosis, apoptosis, hypertrophy, atrophy and synthesis and degradation of the matrix. This process is initiated at the cellular level and growth and adaptation take place due to the formation and removal of cells and matrix. The turnover of different constituents, in turn, affects the mechanical properties of the tissue. Current approaches are based on either reaction-diffusion equations or the concept of volumetric growth through the growth tensor Fg, for which an evolution equation is prescribed. Here we examine here a newly proposed constrained mixture model for growth and remodeling, specifically, we use this new model to present illustrative computations in a representative, transversely-isotropic soft tissue subjected to homogeneous deformations under uniaxial and biaxial loading. The main thrust of the computations is to better understand the consequences of various assumptions for the kinetics of mass production and removal on the mechanics of the tissue.

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Mechanics and Physics of Solid-Solid Phase

(Symposium No. 10)

Organizers:
Dimitris C. Lagoudas, Texas A&M University
Valery I. Levitas, Texas Tech University
Ibrahim Karaman, Texas A&M University

SMA Kinetics Characterization: Micromechanics to Continuum

L. C. Brinson* — Associate Professor

D. Burton* — Graduate Research Assistant

X. Gao* — Postdoctoral Research Associate

A major problem in current modeling of SMAs is difficulty of accurate and tractable prediction of response to complex, non-uniaxial loadings. Although micromechanics approaches can predict grain level and polycrystalline responses more accurately, it is at the expense of intensive computations. Existing continuum level models for multi-dimensional behavior work well for rapid computation and incorporation into finite element schemes, but the kinetics used thus far fail when tested against complicated loading scenarios. This work will demonstrate use of a robust micromechanics based model for shape memory alloy material behavior to guide development of continuum level expressions to describe the kinetics of phase transformation. The micromechanics model used is based on a multivariant system, in which the 24 habit plane variants of each grain in a polycrystalline material are accounted for. This model has been tested against experimental characterization at both the micro and macro scale for simple and complex thermomechanical loadings. Here, the model is used to simulate polycrystalline SMA response to key multidimensional loading scenarios and both the variant level response and the overall strain and martensite fraction state of the system is tracked. The results are then used to develop more appropriate kinetics expressions that can be used within the context of previously developed plasticity-based SMA constitutive laws. The advantage to the approach pursued here is that the existing framework of the previous multidimensional continuum level SMA constitutive laws can be used, along with their finite element implementations, to now obtain accurate response of polycrystalline SMAs under complex, sequenced multiaxial loadings.

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An Absorbing Boundary Condition for 1-D Nonlinear Wave-Type Equations with Application to Impact Loading of Shape Memory Alloy Rods

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P. Popov* Graduate Research Assistant

In this paper an Absorbing Boundary Condition (ABC) method is considered for one-dimensional nonlinear wave-type equations on a unbounded spatial domain. The ABC method considered here is in some respects similar to the infinite element methods for the time domain developed by Astley et. al. for linear problems. Of particular interest is the application of this ABC method to compute stress waves in long rods consisting of nonlinear material and subjected to impact loading. In particular the rods considered here consist of NiTi Shape Memory Alloy (SMA) material. Accurate computational modeling of the stress waves in long SMA rods is important in understanding and predicting the energy absorption and vibration damping characteristics of SMA materials. Consequently, the omputational accuracy and utility of this ABC method when applied to dynamic loading problems is investigated and evaluated.

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A Computational Study of Evolving Phase Fronts in Shape Memory Alloy Thin Films

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Graduate Student Associate Professor Associate Professor

A recently developed one-dimensional (1D) theoretical framework (Stoilov and Bhattacharyya, 2002) is extended to three-dimensional (3D) theoretical framework for describing the thermo-mechanical phase transformations with evolving phase boundaries in shape memory alloys (SMA). The dynamical response of the system is modeled by incorporating the basic conservation laws (mass, linear momentum, angular momentum and energy), and the developed theoretical framework is completed by invoking the notion of continuity of chemical potential at the phase boundaries. The theoretical framework is general enough to incorporate any Helmholtz free energy function of the SMA, and therefore if this function is explicitly known, then so is the entire set of governing equations (including that for the phase boundary evolution).

The theoretical framework is used to study phase front evolution in 2D SMA domains (i.e. SMA thin films) by developing a new numerical algorithm that utilizes finite element method (FEM), phase front tracking and non-oscillatory 2D interpolation. It is shown that the algorithm (O(h2,t2)) is unconditionally stable and adequately accurate by comparing the predictions of the model with the experimental results of Fang, Lu, Yan, Inoue and Hwang (1998) for the shape memory effect and pseudoelasticity in SMA CuAlNi thin films.

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Thermal and Mechanical Characteristics of Ti-Rich NiTi Processed by ECAE at Different Temperatures

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Ni-Ti alloys are the most frequently used shape memory alloys for practical applications due to their outstanding mechanical properties, corrosion resistance and biocompatibility. Severe plastic deformation of NiTi can result in nanostructured (even amorphous) bulk material that has received increasing attention with unique strength and phase transformation behavior. In this study, equal channel angular extrusion (ECAE) was used to severely deform a Ti rich NiTi alloy (50.2 at.% Ti) at various temperatures. ECAE, a severe plastic deformation process, permits the application of a large amount of strain without significant change of sample cross section area. The main difference between ECAE and other severe plastic deformation techniques applied to NiTi (such as rolling) is the amount of strain applied in one deformation pass.

In order to investigate the deformation and resulting shape memory and pseudoelasticity response of stress induced martensite, thermally induced martensite and austenite, rectangular NiTi bars were extruded at two temperatures: (1) below the Mf and (2) above the Af. . Only one pass extrusion was performed because of undesired severe shear and fracture. Differential scanning calorimetry (DSC) was used to determine transformation temperatures (TTs) of extruded materials. It was also utilized to determine the change in TTs with different annealing treatments. Phenomena like recovery, R phase formation, change in TTs with deformation and annealing temperatures were investigated. Microhardness, compression and thermal cycling under fixed stress experiments were used to determine the mechanical properties. Optical microscopy, TEM, and X-ray analysis were used to characterize the resultant microstructures of deformed and annealed materials.

We will present thermal and mechanical characteristics of the severely deformed Ti-rich NiTi. A number of unusual phenomena, such as significant changes in TTs and thermal hysteresis, different deformation mechanisms at different extrusion temperatures and resulting transformation behavior, two-way shape memory and R-phase formation in Ti-rich NiTi, have been observed. The rationale behind these observations will be explained with the help of microstructural evolution and different deformation mechanisms. Combined severe ECAE deformation and subsequent annealing treatments are believed to be more effective ways for marforming and for engineering the thermal and mechanical response of shape memory alloys for a particular application.

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Active Skin for Turbulent Drag Reduction

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Drag reduction for aerial or underwater vehicles has a range of positive ramifications: reduced fuel consumption with the associated economic and environmental consequences, larger operational range and endurance and higher achievable speeds. This work capitalizes on recent advances in active turbulent drag reduction and active material based actuation to develop an active skin for turbulent drag reduction. The skin operation principle is based on computational evidence that spanwise traveling waves of the right amplitude, wavelength and frequency can result in significant turbulent drag reduction. Such traveling waves can be induced in the active skin via active-material actuation. The flow control technique pursued is micro in the sense that only micro-scale wave amplitudes and energy inputs are sufficient to produce significant benefits. The skin is conceived to be adaptive; wavelength, frequency and amplitude would be controlled on-line, in real-time, to produce optimal gains as the flow conditions change.

In this work, two design paradigms for the active skin design have been proposed and analyzed. Several design implementations based on these guiding principles have been developed and their viability has been studied using Finite Element Analysis (FEA) for different applications. Active material actuators, based on Shape Memory Alloys (SMAs) and Piezoelectric materials, provide, in a complimentary manner, a wide range of actuation capabilities, and have been identified as suitable means of actuation, for the different active skin designs. Owing to the micron level amplitude requirements for the traveling wave, a MEMS (Micro Electro Mechanical System) based active skin design, that utilizes thin film SMA/Piezoelectric actuators, has been identified as a promising approach for the realization of a practical active skin.

For preliminary testing and validation of the computational results, a mechanically actuated prototype skin based on cam action has been manufactured using a rapid prototyping machine. The results from the experimental studies would be discussed during the presentation.

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Evolution of Ferroelectric Domain Structures in Thin Film with Structural Defects

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Professor

Many structural defects, such as cracks, grain boundaries, and semi-coherent interfaces, can be described by distributions of dislocations. In the present talk, we introduce an arbitrary spatial distribution of dislocations into a phase-field model for simulating the effect of defects on the nucleation of ferroelectric domains, domain-wall movement and domain structures in thin film. The elastic solutions are derived for elastically anisotropic thin film with an arbitrary distribution of defects and arbitrary domain structures, subject to a substrate constraint. In particular, a [001] orientated PbTiO3 film heteroepitaxially grown on a [001] cubic substrate is considered. The film undergoes a cubic-to-tetragonal ferroelectric phase transition. The nucleation and growth of domains near interfacial dislocations or an interfacial crack are studied. The Curie temperature, the interaction between defects and domain-wall movement, domain structures, and the volume fraction of domain variants are analyzed.

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Energy Minimization, Microstructure and Effective Behavior of Phase Transforming Materials

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The modeling of coherent phase transformations in two phase solids involves the identification of microstructures with minimal energy. We consider two problems, one in single crystals and one in polycrystals. The first problem concerns finding the optimal microstructure and effective properties of a two phase material with arbitrary elastic moduli and arbitrary transformation strain. Previous work in this direction assumed either equal moduli or equal transformation strain.

The second problem concerns shape memory effect (SME) - the ability to recover on heating, apparently plastic deformation sustained below a critical temperature - in polycrystals. The same material might exhibit very different SME as a single crystal and as a polycrystal. In particular many materials exibit good SME as single crystals but little or none as polycrystals. We propose a method to predict the polycrystal behavior when the single crystal behavior is known. For a large class of materials - including materials that undergo cubic-tetragonal transformations - we characterize the class of polycrystals that would exhibit SME. Implications of these results to problems of engineering interest are discussed.

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Micro- and Nano-Scale Engineering
(Symposium No. 11)

Organizer:
Thomas J. Mackin, University of Illinois – Urbana-Champaign

Nanoengineering, Nanotribology, and MEMS: A Multi-Scale Approach to Controlling Friction and Wear

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We have studied the surface topography and nanotribological constitutive behavior of polycrystalline silicon MEMS surfaces with a range of surface roughening and surface chemical treatments. We show that the atomic force microscope (AFM) resolves critical roughness features from the nanometer-to-micrometer scale. We derive surface roughness parameters from the AFM data and use both analytic and numerical techniques to estimate specific contact properties. We find that the roughening procedure leads to smaller contact areas, but also to higher contact pressures that may approach yield values. Measurements of interfacial adhesion and friction with the AFM are fed into our models to develop a predictive understanding of sliding MEMS interfaces. Results are compared with an actual MEMS friction test platform. Our results indicate that surface topographic design in MEMS should integrate surface imaging at the nanometer scale and contact asperity modeling in order to predict optimal surface preparations that minimize adhesion, friction, and wear.

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Mechanical Properties of Carbon-Nanotube/Al2O3 Composites

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Carbon nanotube (CNT) reinforced composites have been touted to possess superb mechanical properties due to the unique structure and properties of carbon nanotubes, but no such materials have been fabricated or reliably tested to date. Here, we present the first results on the mechanical properties of highly-ordered CNT-reinforced ceramic matrix composites. The nanocomposites were produced by the template approach, in which CNT are deposited into a porous alumina matrix formed by anodization of aluminum, and are in the form of thin films (20 mm) on an aluminum substrate. Nanoindentation tests were performed on surfaces both parallel and perpendicular to the longitudinal CNT axis. Indentation marks and associated damage were observed by SEM. Indentation parallel to the CNT axis induced cracks that intersect and deflect at the matrix/CNT interface, indicating interfacial debonding. Indentation perpendicular to the CNT axis induced cracks that show preliminary evidence of nanotube bridging. Indentation at high loads to cause chipping exposed fracture surfaces that exhibit CNT pullout. All of these phenomena indicate that these nanotube composites may function as tough materials. Nanocomposite modulus data obtained from indentation unloading curves were used along with analytic and finite element models to derive the Youngs modulus of the porous Al2O3 matrix (150 GPa) and the CNT (300GPa) parallel to the nanotube axis; the latter values are much lower than typical estimates of CNT stiffness. The fracture toughness for cracking transverse to the CNT (typically a weak direction in CMCs) is estimated to be 7.4 MPa.m, comparable to tough engineered ceramics and much higher than that of bulk amorphous alumina. The crack/nanotube interactions and potentially high residual stresses in these composites may contribute to the high fracture toughness. Overall, the present material system shows some enhanced properties relative to bulk materials and thus holds promise as an advanced coating system for aluminum materials, but is also proving useful for demonstrating composite-like behavior in CNT-reinforced materials and permitting careful studies from which nanoscale material property data can be cleanly extracted.

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A Hybrid Continuum/Tight-Binding Analysis to Study the Effect of Mechanical Deformation on the Electrical Property of Carbon Nanotubes

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Carbon nanotubes show great promise for nano-electronic applications due to their superb electrical properties. Recent experiments, however, show that the electrical conductance of carbon nanotubes may change by two orders of magnitude upon mechanical deformation. This makes carbon nanotubes suitable for NEMS, but may also constitute a potential problem for the reliability of carbon nanotube-based electronics.

We have developed a continuum theory based on the interatomic potential for carbon. This continuum analysis provides the atomic positions of the deformed carbon nanotube. The k-space tight-binding calculations then give the band gap, which is an indication whether the deformed carbon nanotubes has the metal-like or semiconductor-like electrical properties.

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Indentation of Freestanding Membranes With Finite Contact Sizes

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The mechanics of indentation of circumferentially clamped, freestanding, axisymmetric membranes are presented to establish connections between deformation, applied load, and material response. A general large deformation approach is taken that may be applied to a wide range of constitutive behavior and indenter shapes. In the present case we consider a linearly elastic membrane, loaded using a frictionless spherical indenter. The results show strong power-law relationship between radius of contact, the maximum strain in the membrane, the membrane deflection and the applied load. Closed-form asymptotic expressions for deformation in the contact region are presented; a key result is the ability to estimate the maximum indentation strain for a given load. The results are contrasted with existing solutions for point loads that predict infinite indentation strains (yet finite displacements). The solutions are discussed in terms of their potential for extracting mechanical properties from indentation testing of freestanding micro- and nanoscale films and membranes via AFM and nano-indentation. A particular advantage of the solutions is the ability to estimate the contact stiffness of the membrane for a specific amount of strain in the membrane and when probe dimensions are comparable to membrane size.

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Measurements of Polymer Viscoelasticity Using Depth-Sensing Indentation

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For many industry-relevant polymer systems, early times-to-failure can be linked to local chemical and physical degradation, including local changes in mechanical behavior. In multi-component polymer systems, the interphase regions that form at the component interfaces are often found to be the weak links in the material. Even for relatively homogeneous polymers, the behavior of surfaces, which are particularly vulnerable to chemical and mechanical stresses, and thin films are of particular importance in numerous applications. Thus, development of techniques to characterize microscale and nanoscale mechanical properties is important for improving the performance of these materials. Currently available systems that can be used to perform suitable measurements include scanning probe microscopes and depth-sensing indenters. Scanning probe microscopes have several important capabilities such as low-load sensitivity and extremely sharp tips for excellent lateral resolution, and their imaging capabilities are often unmatched. However, quantitative measurements of mechanical properties are limited by potentially large experimental uncertainties, and appropriate experimental control over important test parameters is generally not attainable.

Recent advances in depth-sensing indentation (DSI) systems, sometimes called nanoindenters, allow for extensive control over experimental variables, and the addition of dynamic testing capabilities has improved sensitivity at low load levels. However, lingering questions remain regarding system calibration methods, and the application of traditional nanoindentation measurements to polymeric materials has significant limitations. In this presentation, key issues in characterizing viscoelastic behavior of polymers using nanoindentation will be examined. Experimental methods for measuring creep and stress relaxation behavior, as well as dynamic mechanical behavior, with a nanoindenter will be discussed. Examples of such measurements will be presented for a range of polymer chemistries.

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Mechanical Characterization of Ultra Thin Nano-Crystalline Metal Films by MEMS Instruments

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The current limitation in studying mechanical properties of nano-crystalline thin films is the lack of instrumentation that allows both qualitative and quantitative in-situ investigations. Here we present a MEMS based methodology to apply known forces on material samples of free standing thin films (20 nm and higher) and measure corresponding displacements of the samples. The method allows in-situ observation of the samples in SEM or TEM while their stress-strain response is being measured. Thus, it allows to explore the mechanisms of deformation and failure of nano scale materials under a wide variety of environmental conditions. We demonstrate the methodology by carrying out uniaxial tensile experiments on 30-200 nm thick free standing aluminum and gold films in-situ in an SEM. The grain size of the films is in the range of 10-100 nm. We find, with decreasing grain size: (1) elastic modulus decreases, and (2) material shows non-linear elastic response. We attribute the large proportion of grain boundaries in nano-grained materials as contributing to these two observations. We propose the following model: the atoms in the grain boundary are disordered compared to those within the grains. Thus, some atoms are further apart from one another compared to the equilibrium separation between them. Hence, local tensile stress develops in some regions. In order to maintain force equilibrium, some regions are under compressive stress where the atoms are closer to each other compared to equilibrium inter-atomic distance. Since the inter-atomic force-distance relation is steeper under compression than under tension, hence the effective elastic modulus of the grain boundary is lower than that within the grains. Under tensile strain, the atoms in the local tensile region move further apart from one another, whereas, the atoms in the compressive region approach or exceed the equilibrium inter-atomic distance. Thus, the force response softens with increasing strain. With unloading, the grain boundary returns to initial configuration without any energy dissipation. As the grain size decreases (to 50 nm or below), (a) it becomes energetically unfavorable to sustain dislocations within the grains, and (b) the volume fraction of grain boundary increases. Both (a) and (b) allow most of the deformation to be accommodated by the grain boundaries giving rise to lower effective elastic modulus and non-linear elastic response.

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Thermomechanical Model Predictions for the Response of Adhered MEMS Cantilevers Due to Laser Heating

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Developments in micro- and nanoscale engineering require an understanding of surface and interfacial phenomena. The surface area-to-volume ratios result in surface forces being more significant in micro- and nanoscale systems than in macroscale systems. In microelectromechanical systems (MEMS), surface forces can lead to adhesion between structures and the underlying substrate or adjacent parts, which then results in device failures. Disadvantageous adhesion restricts design rules, manufacturing processes, operating environments, and the transfer of technology from the laboratory to the marketplace. One method for repairing adhered MEMS structures uses pulsed laser irradiation. A thermomechanical model for adhesion reduction due to laser heating has been developed and shown to agree with experimental results for polycrystalline silicon (polysilicon) MEMS cantilevers.

Using fracture mechanics based methods, the thermomechanical model considers the interface between an adhered cantilever and the substrate as a crack. When a microcantilever is irradiated by a laser, the cantilever is heated to a temperature higher than that of the substrate. The temperature difference between the microcantilever and the substrate increases the strain energy release rate. The crack will grow when the strain energy release rate exceeds the surface adhesion energy. Predicted crack lengths using the model are in good agreement with those measured experimentally for polysilicon microfabricated cantilevers irradiated with a 532 nm Nd:YAG laser. The model has also been used to examine the effects of surface adhesion on the achievable crack lengths during single and multiple pulse laser operation.

In order to determine the effectiveness of the laser repair process for a given microsystem, the optical, thermal, and mechanical properties must be considered. The optical and thermal properties dictate the amount of temperature increase in a structure for a given laser operating condition and the amount of time the structure remains at this elevated temperature. The mechanical properties and the structural dimensions determine the increase in the strain energy release rate for a specified temperature difference. The laser repair process has been investigated for various cantilever geometries and materials. By using the model, the likelihood of successful laser repair can be predicted and an appropriate laser selected.

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Mechanical and Constitutive Properties of Thin, Soft Layers: Preliminary AFM Experiments and Related Modeling

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Cell mechanical properties and constitutive behavior play important roles in the function of biological materials. Cell performance, its interactions with surrounding media, and its response to stimuli are all closely related to the macro- and micromechanical properties of the cell. Cell mechanical properties and constitutive behavior provide a direct link between cell deformation and mechanical work. Therefore, characterizing cell mechanical properties becomes a very important goal, particularly in cells with a strong mechanical function such as muscle cells.

We will report preliminary results from this line of research using a model biological system (a thin vitellin layer) and atomic force microscopy (AFM) for static and dynamic indentation tests. Complementary modeling efforts for the indentation processes will also be reported. The experimental focus is to observe material linear, nonlinear, and viscoelastic effects, as well as contact adhesion components, under both small and large indentations. We use various AFM modes and examine repeatability of the data, and therefore provide direct experimental evidence of the contact behavior. Mechanical properties and constitutive behavior of the materials are extracted using contact models to interpret the AFM data. The key result is the sensitivity of mechanical property calculations to the details of the experiment and the contact models. We discuss the implications of contact model choice on mechanical property identification, and focus specifically on the potentially large errors involved with using standard linear elastic contact modeling approaches.

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Static Dielectric Constant of Particulates Determined with Electroacoustic and Attenuation Spectroscopy

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Vahit Atakan* Graduate Student
Richard E.Riman* Professor

Both electroacoustic and attenuation spectroscopy could be used to determine the particle size distribution of particulates material. The particle size distribution data obtained with the electroacoustic spectroscopy was strongly dependent on the static dielectric constant of the particulates, while the particle size distribution data obtained with the attenuation spectroscopy was independent of the static dielectric constant of the particulates. The theories of the electroacoustic and attenuation spectroscopy were reviewed with the emphasis on the correlation between the particle size and the dielectric constant. The static dielectric constant of particulates can be assumed as a value at which the particle size data obtained via the electroacoustic technique is identical to the one obtained via attenuation spectroscopy. Three particulate materials, BaTO3, Al2O3 and PZT(lead zirconia titanite), were taken as examples in this paper. The particulates were dispersed into deionized water and measured with AcoustoSizerII (Colloid Dynamics, RI). The particulates were compressed into a disk and the dielectric properties were also measured with HP 4284A LCR meter. The static dielectric constant obtained with HP LCR meter agreed well with the one obtained from the electroacoustic technique.

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Nanoscale Science and Technology
(Symposium No. 12)

Organizer:
Akhlesh Lakhtakia, The Pennsylvania State University

Controlled Column Tilt Angle Using Non-uniform Substrate Rotational Speed in Glancing Angle Deposition†

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Thermal vapor beam deposition on a fixed substrate with glancing incident angle results in tilted nanocolumnar thin films. The angle of tilt β increases as the incident angle of vapor beam θ increases and in general $\beta < \theta$ due to shadowing effect. It was also shown that it is possible to control the tilt angle β of the columns by fixing the vapor incident angle θ while varying the phase and speed of substrate rotation [1]. We have explored in more detail the growth of a columnar film with a desired tilt angle by changing one of the three parameters: rotational speeds in two angular sectors in one revolution, the magnitude of angular sector, and incident angle θ. We set the rotational speed to be ω_1 in an angular sector of ϕ and change the rotational speed to ω_2 in the remaining angular sector of $2\pi - \phi$. We demonstrated this control of tilt angle using thermal evaporation of Co on Si substrates. The columnar films were imaged by a field emission scanning electron microscopy (FESEM) and the tilt angles were obtained from the cross-sectional SEM images. We derived a simple equation that relates the equivalent angle of incident vapor θ', to the three parameters: ω_2/ω_1, ϕ, and θ. As the substrate rotates uniformly ($\omega_2 = \omega_1 = \omega$) one gets $\beta = 0$ or vertical columns. Otherwise, tilted cobalt columnar films are sculptured. The measured tilted angle $\beta < 40^o$ in our experiments for $\theta = 65^o$. The calculated tilt angles also compared reasonably well with those obtained from films grown under wide ranges of ω_2/ω_1, ϕ, and θ. This control of tilt angle becomes useful for growing 3D structures if one cannot change the angle of incident vapor beam but can easily change the rotational speed.

[1] K. Robbie, J. C. Sit, and M. J. Brett, J. Vac. Sci. Technol. B 16, 1115 (1998).

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Nominal Microstructure–Based Model for Chiral Sculptured Thin Films: Dielectric and Bianisotropic Properties

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A nominal structure–property relationship model for a chiral sculptured thin film infiltrated with a chiral fluid, based on ellipsoidal topology is presented. The effect of the constitutive and microstuctural parameters on the optical response of the chiral sculptured thin film is thereby explored. Specific stucture–property relations are developed. To calibrate the model, a chiral sculptured thin film is fabricated from patinal titanium oxide using the serial bideposition technique. Axial transmittance spectrums are measured over a spectral region encompassing the Bragg regime for axial excitation. The same spectrums are calculated using the nominal model and the parameter space of the model is explored for best fits. An ambiguity arising on calibrating the nominal model against axial transmittance measurements is shown to be resolvable using non–axial transmittance measurements. Its resolution is also demonstrated through the infiltration of the chiral sculptured thin film by a chiral fluid.

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Retardation of Oxidation in Co Nano-Columns

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The Co nano-columns with ~18 nm diameter and ~100 nm thickness were prepared by the glancing angle deposition (GLAD) technique at 85° incidence angle with substrate rotation [1,2]. The properties were studied ex situ by scanning electron microscopy (SEM), atomic force microscopy (AFM), scanning tunneling microscopy/spectroscopy (STM/STS), and X ray photoelectron spectroscopy (XPS). The nano-columns were observed by SEM, AFM, and STM to be vertical with smooth tops, whereas the conventional polycrystalline film exhibits a granular structure with high density grains of ~28 nm as observed by AFM. The current-voltage (I-V) spectrum of a single nano-column shows a linear variation of the tunneling current under a bias voltage applied to the sample in contrast to that of a non-linear behavior for the conventional film. A non-oxidized Co peak at -0.7 eV corresponding to the 3d valence electrons was observed in the dI/dV spectroscopy of the individual nano-column. This peak was absent in the dI/dV of a conventional film. It is argued that a retardation of the oxidation (CoO and Co_3O_4) in the Co nano-column is due to the lack of grain boundaries in the isolated nano-columns. This is contrary to the fast oxidation via grain boundaries that were commonly observed in the conventional polycrystalline metal films.

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Investigation of the Stress Corrosion Cracking, Corrosion Fatigue and Localized Corrosion Resistance of Conventional and Nanostructured Al-Mg Alloys

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The corrosion behavior of nanocrystalline Al-Mg based alloys is being investigated and compared to their conventional counterpart 5083(H111). Specifically, the resistance to stress corrosion cracking (SCC) and corrosion fatigue (CF) is being studied. The objective of this investigation is two-fold: obtaining both (1) design data and (2) fundamental information on the mechanisms of corrosion in nanostructured Al-Mg based alloys.

Design data that the program is generating includes the SCC susceptibility of the nano-Al-Mg alloys compared to their conventional counterparts in artificial seawater and natural seawater. The pitting densities, average pit depths and crack initiation time were measured under different loading conditions after alternate immersion in artificial seawater and ocean front exposures. For non-loaded samples, residual strength values were compared for both alloys after time intervals of 2 weeks, 1 month, 2 months and 4 months. Scanning Electron Microscopy (SEM) was used to analyze the fracture surface of the failed specimen after removal at selected time intervals and tensile testing. Locating the initiation of fracture, type of failure (transgranular or intergranular) and cause of failure was the focus. S/N curves were generated under fatigue loads for the nanocrystalline Al-Mg based alloy and the conventional counterpart 5083, in air and seawater. A range of microstructural experiments were aimed at identifying the role that the grain boundaries play in altering the localized corrosion mechanisms of the alloys. The results of this investigation will provide the necessary information regarding the role that ultra-fine microstructures play in their degradation in marine environments.

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Particle Systems
(Symposium No. 13)

Organizers:
Virendra M. Puri, The Pennsylvania State University
J. Guadalupe Arguello, Sandia National Laboratories

Anisotropy in Powder Compaction: Methods for Analysis and Testing

Arthur L. Gurson*

Principal Technical Staff

Most numerical simulations of plastic flow in powder compaction use a yield function / plastic potential which is isotropic, and is a function of the first two invariants of stress. The micromechanics of die compaction, with the larger deformation in the axial direction, suggest that the compact may not in fact be isotropic. This could introduce a substantial inaccuracy. In this work, a yield function of the above type is modified for anisotropy by applying coefficients to the stresses that are related to the deformation history. Methods are presented to estimate these coefficients using an adaptation of the compaction plane model of Fleck (1995) and to measure these coefficients based on compression of cubic specimens in a die with a square cross section. The results suggest that data from anisotropic compaction tests can be projected to a baseline isotropic case, which can then be used to project back to other anisotropic cases. Material models for powder compaction are usually calibrated to the results of triaxial compression tests, in which the yield points of compacted powders are measured at various ratios of axial and radial stress. A method for performing these tests is presented in which the powder is first die compacted to a specified density, then recompressed at the triaxial condition. The powder is contained in a metal sleeve, which in the first step is contained in a rigid die. The first compaction is thus die compaction, with zero radial displacement. Using special fixturing, the punches and sleeve are then ejected from the die. The powder is then compressed again to a specified specimen height. The punch load provides the axial stress, and plastic yield of the sleeve provides the radial stress. Radial stress at yield can be varied by choosing different wall thicknesses and/or materials for the sleeve. Punch displacement and radial expansion are used to compute a strain rate vector. Because the specimen is die compacted prior to the triaxial test, the specimen should be anisotropic. Methods discussed previously can be used to project the triaxial data points to an isotropic equivalent. This triaxial test method was developed for several reasons: The cylindrical specimens require no machining, which is important for weak compacts. Operator contact with the powder is minimized, which may be a factor when testing toxic materials. The powder can be contained in the sleeve, so accountable material is more easily kept and recovered. Only axial force and displacement need to be recorded, so standard testing machines can be used.

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Properties of Granulated Ceramic Powders in Hydrostatic and Triaxial Compression

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As part of an effort to simulate ceramic powder compaction using finite-element modeling, the mechanical properties of seven granulated ceramic/binder powder systems were measured. The powders and pressed compacts of those powders were characterized at pressures up to 69 MPa (10Kpsi) using hydrostatic and triaxial compression tests adapted from the soil mechanics field. The pressure-density relationship for each powder was determined in isostatic compression. Youngs, bulk, and shear modulus, and Poissons ratio were determined as a function of pressure. Powder yield and failure strengths were determined under deviatoric loading. Together, the hydrostatic and triaxial compression tests produced the necessary data to define the shear failure and hardening cap surfaces that comprise a cap-plasticity constitutive model for powder compaction.

For all seven powders examined, the Youngs, bulk, and shear moduli all increase linearly with pressure up to 10 MPa. Poissons ratio is not pressure dependent. The cohesion of all seven powders is uniformly low, and the shear failure surface is linear over the pressure range studied. The angle of internal friction of the powders ranges from 25-35 degrees. Ceramic powders that are stronger in triaxial compression have a higher angle of internal friction, and pressibility improves with decreasing angle of internal friction.

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Quantification and Constitutive Modeling of Visco-elastoplastic Properties of Ceramic Powders Using a Cubical Triaxial Tester

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A medium pressure (up to 42 MPa) flexible boundary cubical triaxial tester (CTT) was developed during this research. Two types of undrained triaxial tests (hydrostatic triaxial compression test and conventional triaxial compression tests) were done on two spray-dried ceramic powders alumina and ferrite. The fundamental stress-strain engineering parameters (such as bulk modulus, shear modulus, compression index, swelling index and time-dependent properties) of the powders were determined at different isotropic pressure values (2 to 35 MPa) and loading rates up to 21 MPa/minute. The bulk modulus, shear modulus and failure stress values of the powders increased with increasing isotropic pressure but decreased with increasing loading rate. Statistical correlations at 95% confidence level were developed between loading rates, engineering parameters and isotropic pressure of compression. The compression, shear and failure data from the CTT was also used to develop a set of visco-elastoplastic constitutive equations for dry powder compression under different loading rates. These constitutive equations were developed using critical state theory, modified Cam-clay model and Adachi-Oka model as backgrounds. The critical state line was modeled using a power-law equation and high R-square values (greater than 95%) were obtained. Also, the work hypothesis was modified to determine the shape of the moving yield surface during powder compression.

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Investigating Axial and Radial Powder Movements during the Compaction of Pharmaceutical Excipients

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Powders in their granular form can be compacted within specifically shaped punches under high pressure to produce the desired compacted shape. For example being either curved or flat faced tablets. The elucidation of the mechanisms of tabletting is of fundamental importance to a wide variety of interests; for example in powder metallurgy, the ceramic industry, explosive filling, catalyst manufacture and medicinal tabletting (Train, 1957). Many techniques for densification have been developed and optimised to suit particular material properties and product requirements.

The application of pressure to a powder, within the confines of a punch and die, results in an increase in powder density and the formation of a solid compact.

As a powder is compacted in a die, various zones are subject to differing intensities of pressure and shear. This is due to the frictional properties of the powder and tooling and will results in differing density and flaw distributions within the tablet. These resulting inhomogeneities give rise to the potential for subsequent poor tabletting performance such as capping and lamination

The coloured layer technique was used to assess the density distributions within the tablet similar to the method used by Train with vertical and horizontal coloured layers for both curved and flat faced tablets. A laser profilometer was also used to assess the surface roughness of the specimens. Results revealed high levels of inhomogeneity and density distribution for both curved and flat faced tablets with the curved faced tablets being susceptible to lamination. It was apparent that large amounts of axial and radial powder movements were taking place more so, at higher compaction pressures. Surface topography revealed that the surface of the tablets changed after the compaction process.

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Maximum Packing Fraction Predicted on the Basis of Particle Size Distribution and Determined via the Rheological Measurement

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An analysis technique for calculating the maximum packing fraction has been developed on the basis of Sudduths methodology (R.D. Sudduth, J. Appl.Poly. Sci.,48, 37-55(1993)). The number geometric mean, number geometric standard deviation and the particle packing configuration were needed for calculation. The former two parameters could be determined via particle size analysis instruments, and the latter one was assumed either as the loose random packing or as the dense random packing in consideration of the wide particle size distribution range of the sample used in this study. A series of samples of different particle weight loading was prepared and the viscosity of each sample was determined in a wide shear rate range (0.01 to 1000 /s). The reciprocal viscosity against the particle volume fraction was plotted and fitted by a first order polynomial. The line was extrapolated to the point where the reciprocal viscosity is zero and the volume fraction at this point was claimed as the maximum packing fraction. The titanium dioxide particulates with median particle size 300 nm dispersed in a polymer (versa flow, Shamrock, NJ) were studied. The calculated maximum packing fraction was 0.6 and the experimental result was 0.5. The difference between the experimental result and calculation was attributed to the highly viscous medium in which the particles were dispersed.

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Continuum-Based FEM Modeling of Ceramic Powder Compaction

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Software has been developed and extended to allow finite element (FE) modeling of ceramic powder compaction using a cap-plasticity constitutive model. The underlying, general-purpose FE software can be used to model even the most complex three-dimensional (3D) geometries envisioned. Additionally, specialized software has been developed around this framework to address a general subclass of axisymmetric compacts that are common in industry. The expertise required to build the input deck, run the finite element code, and post-process the results for this subclass of compacts is embedded within the specialized software. The user simply responds to a series of prompts, evaluates the quality of the FE mesh that is generated, and analyzes the graphical results that are produced from the simulation. The specialized software allows users with little or no FE expertise to benefit from the tremendous power and insight that FE analysis can bring to the design cycle. The more general underlying software provides complete flexibility to model more complicated geometries and processes of interest to ceramic component manufacturers but requires significantly more user interaction and expertise.

This work was supported by the US Department of Energy under contract DE-AC04-94AL85000 and through a DOC/EDA grant from AMMPEC. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the US DOE.

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A Finite Element Study of Particle Fragmentation During Compaction of Particulate Materials

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Recently we have simulated the compaction of powders using finite element descritization of individual particles. The computational cost of the solution restricts the application currently to 2-D problems but allows great flexibility in terms of material model, contact conditions and particle geometry. In this paper we utilise similar simulations to understand the problem of particle fragmentation during compaction of brittle systems. The origin of tensile principle stresses in a primary compressive deformation process are identified, and it imprortance in the various stages of compaction is assessed.

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Simulation of the Die Compaction and Sintering Process with Finite Element Method

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The research effort oriented towards the modeling of metal powder sintering is to accurately predict the distortion of sintered part, which is mainly due to the differential shrinkage of green compact. Therefore, it would be beneficial to combine the simulations of die compaction and sintering together. Firstly, the pressing and spring-back are simulated during die compaction and ejection. The porous elasticity model and modified Drucker-Prager/Cap plasticity model are used in the static pressing problem. Shape change, residual stress and density distribution data are transferred into the sintering simulation as initial conditions. Secondly, the densification and distortion of stainless steel 316L powder compacts are investigated during sintering. The power law creep model is used to simulate the viscoplastic behavior under sinter forging. The diffusional flow model is used for pressureless sintering. A combined model is created for a more general situation. The grain growth equation is empirically determined by image analysis on metallographs of sintered cold isostatic pressing (CIP) samples. The definition of viscosity in each viscoplastic model is discussed. A cyclic loading dilatometer is used to in situ measure the corresponding viscosity during free sintering and sinter forging. The simulation results of axial shrinkage and shape distortion are compared with experimental data, and the further development direction of the constitutive law is discussed.

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Experimental, Simulation and Nonlinear Dynamics Analysis of Galton's Board

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Denis L. Blackmore† Professor
Liam Buckley* Graduate Student
Mark Johnson* Graduate Student
Chris Oshman* Graduate Student

The motion of a small object (particle) moving through an array of rigid obstacles, generally known as Galtons board is investigated experimentally, by physical experiments, particle dynamics simulation and by dynamical systems theory analysis of a simple approximate model. High sensitivity of this to a number of parameters such as particle properties, geometry of the obstacle arrangement, release conditions and gravitational strength is a hallmark of Galtons board dynamics.

Physical experiments are performed using small aluminum, brass and stainless steel balls using a mechantronic system that allows fully automated data collection. Statistics on mean velocities and diffusivities are determined from the data. Realistic particle dynamic simulations are also run and the statistical values obtained for several quantities are compared with those deduced from experiments.

Finally, a discrete dynamical systems model of the form xn+1 = F(xn, n) is developed for Galtons board dynamics using standard elastic and inelastic models for the particle-pin interactions. Here xn is the horizontal coordinate of the particle as it passes through the nth row in the pin configuration on the board, where the rows are ordered from the top down. Predictions based on this mathematical model are found to compare favorably with those obtained experimentally and by simulation. In addition, careful analysis of the dynamical systems model reveals the existence of bifurcations and chaotic regimes.

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A Variographic Approch to Continuous Mixing of Particulate Material

Ali Ghaderi*

M.Sc.

Requirements for large throughputs with a constant composition in an uninterrupted process represent an expanding sector in process industry. This has resulted in an increased interest in continuous mixers/ mixing. A good characterization of this type of mixers is necessary in order to achieve optimal mixture quality.

The process of continuous powder mixing is analysed in the light of P. M. Gy's sampling theory. The function of mixer and quality of the mixture is related to Gy's concept of Heterogeneity.

G. Matheron introduced the variogram function for studying the sampling of ore bodies in 1960. It was later adopted by Gy in studying the time-based chronological series. In 1981, Gy published a paper on bed-blending where he applied the variogram function to analyse the blending process. Based on his results, it is shown that input and output variograms are useful tools for characterizing the performance of a continuous mixer.

Variance Reduction Ratio (VRR) was introduced by P.V. Danckwerts in 1953, in order to characterize the continuous flow systems. In 1993, R. Weinektter and L. Reh showed that the final homogeneity of solid mixtures is limited. They proposed a modification of Danckwerts' formula which takes into account the above mentioned limitation. Based on variographic analysis and results from linear system theory, a new formula for calculating the VRR is proposed. This formula confirms the result by Weinektter and Reh and is easier to calculate. It also explains the nature of deviation from Danckwerts formula and ties that to the particulate structure of the material.

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Modeling the Dynamics of Fabric in a Rotating Horizontal Drum using the Discrete Element Method

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Carl Wassgren*
Assistant Professor

In order to provide a tool for designing more efficient methods of mixing fabric, a simplified discrete element model was developed for modeling fabric dynamics in a rotating horizontal drum. The geometry is essentially a horizontal ball mill, but with the media consisting of fabric rather than rigid particles.

Because modeling the interactions between actual pieces of fabric is quite complex, two simplified models were developed. In the first model, individual pieces of bundled fabric are represented by spherical particles. This model is essentially a ball mill. The second model consists of a string of spherical particles connected together to form fibers. The goal of the fiber model is to capture the deformation of unbundled fabric and incorporate the possibility of tangling between fabric elements.

The simulations are used to investigate the particle (fiber) kinematics, the power required to drive the rotating drum, the power dissipated through normal and tangential contacts, the forces acting on the drum, and the forces acting on individual particles (fibers). A parametric study was performed to investigate the effects of fill level, rotation speed, friction coefficient, coefficient of restitution, and baffle geometry.

The simulation results indicate fill percentage, rotation speed, and friction coefficient play a significant role in the particle (fiber) dynamics. The existence of baffles only plays a role at low fill percentages. Particle size, baffle size, and coefficient of restitution have a relatively weak influence. The trajectories of short fibers are similar to those observed for the spherical particles; however, the ratio of normal-to-tangential forces is different.

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A Parametric Pressing Study Using A Plastic-Bonded Explosive

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Pressed plastic-bonded explosives, PBXs, are commonly used by defense and private industry. PBX 9501 is composed of HMX crystals held together with a plastic binder softened with plasticizers. The detonation behavior of any explosive is very dependent upon its density, with the desire to have a uniform, high density throughout the explosive component.

A parametric study has been performed pressing PBX 9501 hydrostatically and uniaxially. The effects of several pressing parameters on the bulk density profile, as well as mechanical properties, have been measured. The parameters investigated include pressure, temperature, number of cycles, dwell time, rest time, sack thickness, and particle distribution and size. Density distributions within the pressed explosives were also compared.

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Polymer Mechanics

(Symposium No. 14)

Organizers:
I. Joga Rao, New Jersey Institute of Technology
Grama Praveen, General Electric Corporate R&D

Flow Characteristics of a Multiconfigurational Viscoelastic Fluid in an Orthogonal Rheometer

A. R. Srinivasa*

Assistant Professor

This work deals with the flow characteristics of a class of non-simple viscoelastic fluid models developed by Rajagopal and Srinivasa(1999). The central feature of these models is that the stress response is elastic from changing natural configuration with the viscous dissipation occurring due to changes in the natural state. The considered class of models are characterized by three independent parameters that represent respectively the elasticity, the viscosity and the shear thinning index.

The stress relaxation response of the material is compared with experimental data reported by Bower et al. (1987) for polyisobutelene in cetane, and parameters that fit the data are calculated. The flow of such a fluid between parallel disks rotating about non-coincident axes (the orthogonal rheometer) is then studied. It is shown that the assumed velocity field leads to a system of second order nonlinear ordinary differential equations (Rajagopal 1982).

A parametric study is then undertaken to see the effect of the various material, geometrical and flow parameters on the flow characteristics. It is observed that inertial effects and shear thinning effects are roughly complementary in the range of parameters considered. While it is well known that boundary layers occur in these flows due to inertial effects, it is demonstrated that these boundary effects are insensitive to the Reynolds number but rather are determined by the absorption number. Finally, in the range of parameters that are commonly observed in such rheometers, it is shown that neglect of inertia causes significant discrepancies in the calculation of the boundary shear rates.

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On the Mechanism of Stress Production and Relaxation in Polymeric Melts

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Assistant Professor

A new framework is developed to describe stress production and relaxation in dense polymeric systems. Stress is traditionally defined on the molecular scale, with the chains being regarded as entropic springs. In this view, the polymeric chains are considered to be always in tension and stress is due exclusively to bonded interactions along the chains. Stretching the chains leads to a retractive force of an entropic nature. Non-bonded interactions between atoms belonging to neighboring chains are considered to lead to hydrostatic stress only.

The new description is defined on the atomic rather than on the molecular scale. It takes into account all (bonded and non-bonded) interactions, and makes no apriori assumption about the behavior of any component of the system. Since it is defined on the atomic scale, the description captures all fast and slow relaxation modes that correspond to short and long wavelength perturbations, respectively. It is therefore equally applicable to small and large volumes of material and to short and long chains.

An overview of the new framework will be presented in the talk. The emphasis will be put on new results and on the parallel between the molecular scale and the atomic scale description of stress. It will be discussed which assumptions made in the molecular theory are justified by atomistic simulations results and which are not. It is shown that both theories are in qualitative agreement with the experimentally observed physical picture.

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A Thermomechanical Framework for the Glass Transition Phenomenon in Certain Polymers

K. Kannan* I.J. Rao† K. R. Rajagopal‡

Student Professor Professor

A thermodynamic framework is developed to describe a polymer melt undergoing glass transition that takes into account the fact that during such a process the underlying natural configurartions (stress-free states) are continually evolving. Such a framework allows one to take into account changes in the symmetry of the material, if such changes takes place. Moreover, the framework allows for a seamless tansition of a polymeric melt to a mixture of a melt and an elastic solid to the final solid state. The efficay of the model is tested by studying the fiber spinning problem for polyethylene terephthalate and the predictions agree well with the experimental results.

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Modeling of Bimodal Networks: Incorporating Network Morphology into an Analytical Constitutive Model

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Assistant Professor

Bimodal polydimeythlsiloxane elastomers have long exhibited properties that vary sharply with the materials composition. Recent developments in the investigation of how the underlying microstructure changes with composition have allowed researchers to postulate and examine links between various network morphologies and the bulk materials behavior. This work combines results of computational simulations of the gelation of bimodal PDMS and an analytical theory of the elasticity of bimodal elastomers, both developed by the author, to construct a constitutive model that incorporates the micromechanics of network effects as functions of the network composition. In particular, the work addresses the effects of doubled connections, computationally predicted reinforcing topologies whose populations follow trends seen experimentally in the enhancement of the ultimate strength of the material. The inclusion of these doubled-connections is shown to affect the chain-level orientation response of the network as measured by birefringence in a manner similar to results seen experimentally. The model, based on Langevin statistics of the freely jointed-chain, also solves the longstanding problem of enforcing kinetic equilibrium between the materials constituents in closed form. The analysis yields a non-affine, large deformation constitutive model whose efficacy is shown across a range of materials.

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Mechanics of Shape Memory Polymers

I. J. Rao*

Assistant Professor

Shape memory polymers are novel materials that can be easily formed into complex shapes, retaining memory of their original shape even after undergoing large deformations. In this paper, we develop constitutive equations to model the thermo-mechanical behavior of crystallizable shape memory polymers. This is done using a framework that was developed recently for studying crystallization in polymers. The constitutive equations are formulated in a full thermodynamic framework using the notion of multiple natural configurations. Here, we outline the main components of such a model and investigate its response for a crystallizable shape memory polymer undergoing a typical thermo-mechanical cycle. The results of the model compare favorably with experimental observations.

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Start Up of a Nonlinear Viscoelastic Material in an Orthogonal Rheometer

A. S. Wineman*
Professor

K. R. Rajagopal†
Professor

The orthogonal rheometer is an instrument that is used to characterize the material properties of non-Newtonian fluids as well as nonlinear elastic solids. The instrument essentially consists of two parallel plates that rotate about non-coincident axes. In the case of fluids, the plates rotate with the same constant angular velocity. For any simple fluid, it is possible to find a velocity field for steady flow that satisfies the equations of motion without neglecting the inertial terms. The interaction between inertia and nonlinear materials properties has been studied for a number of fluids. Interesting boundary layer structures develop adjacent to the plates with a core region of fluid rotating as a rigid mass. In the case of nonlinear elastic solids, the plates have a fixed angular displacement and the equilibrium states have been characterized.

In the present work, we study the start-up problem for flow in an orthogonal rheometer when the plates suddenly go from rest to the same angular velocity. The time dependent deformation of a viscoelastic material is determined that satisfies the equations of motion without neglecting the inertial terms. The results enable the dependence of the evolution of the steady state deformation to be related to the viscoelastic and inertia properties of the material.

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Constitutive Modeling of Sand Asphalt

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Forsyth Chair Professor

The majority of the studies devoted to modeling asphalt pavements are directed towards simulating failure mechanisms of asphalt bound granular materials and can hardly be classified as constitutive specifications. The tests conducted to characterize these failure mechanisms do not take into account the diverse response characteristics of different types of asphalt mixtures. They use shift factors of the order of 3000 percent when comparing field performance data to the laboratory experiments. In this study, we propose a rigorous thermodynamic framework for constitutive modeling of sand asphalt. Sand asphalt differs from the traditional asphalt concrete mixture in its mechanical response in that it exhibits a viscoelastic fluid-like behavior even under normal working temperatures. This is due to the use of fine aggregates and asphalt in larger proportion when compared with asphalt concrete. Also, sand asphalt differs from asphalt concrete in that they are compacted to relatively higher initial air voids of the order of 10 percent. Due to the inherent differences in the materials used in the manufacture of sand asphalt in comparison with asphalt concrete, the mechanism of failure could trace a different path for identical loading and environmental conditions. This necessitates a clear specification for the constitutive properties of sand asphalt as well as for any other asphalt bound mixtures.

Using a recent framework that associates different natural configurations (for example stress-free configurations) with distinct internal structures of the body, we model sand asphalt. In contrast to our earlier study on asphalt concrete wherein we used a constrained two constituent mixture for modeling asphalt concrete, we assume sand asphalt to be a homogenized single constituent. This reasoning is motivated by the fact that very fine aggregates are used in sand asphalt and hence a tendency to resist deformation through the development of a stiff aggregate skeleton as normally exhibited in an asphalt concrete layer is absent in sand asphalt. Assuming appropriate choices for the Helmholtz potential, rate of dissipation and other thermodynamic variables, we derive the constitutive model for sand asphalt. We compare the predictions of the model with the experimental data related to the creep test of sand asphalt available in the literature.

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S. Nemat-Nasser Symposium

(Symposium No. 15)

Organizers:

John R. Willis, Cambridge University
Mohammed Zikry, North Carolina State University

Stress Amplification in Thin Ligaments

X. Markenscoff*
Professor

Stress amplifies singularly in thin ligaments, i.e., vanishingly small regions between cavities, cavities and edge boundaries between cracks, and between rigid fibers under different loadings, including traction at infinity, body forces, thermal loading or dislocation (slip) loading. Analytic solutions and beam theory approximation are discussed.

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Second-Order Homogenization Estimates for Viscoplastic Polycrystals

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Professor Research Assistant

The recently developed "second-order" homogenization method [1] is adapted to viscoplastic polycrystals and used to compute the effective response of certain special classes of isotropic polycrystals. The method itself reduces to a simple expression requiring the computation of the *averages* of the resolved shear stresses (or strains), as well as *the covariance of the fluctuations* of these shear stresses (or strains) over each crystal orientation, within a suitably defined "linear comparison polycrystal." Therefore, the method not only allows the determination of the effective behavior of the polycrystal, but, as a byproduct, also yields information on the heterogeneity of the stress and strain fields within the polycrystal. An application of the method will be given for a model two-dimensional, isotropic polycrystal with power-law behavior for its constituent grains. The resulting predictions for the effective behavior will be compared with the corresponding predictions of other recently proposed estimates and bounds. The associated information on the resolved shear stresses and strains, as well as their fluctuations, will also discussed in some detail, particularly, for the purposes establishing the effects of grain heterogeneity and nonlinearity on the variability of the stress and strain fields within the polycrystal. Such information may have potentially significant implications, for example, in the development of damage within the polycrystal, as well as in texture evolution during finite deformation processes of such materials. Finally, time permitting, some preliminary results will be given for three-dimensional FCC polcrystals.

References

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Boundary-Layer Corrections for Stress and Strain Fields in Randomly Heterogeneous Media

R. Luciano*
Professor

J. R. Willis*
Professor

This presentation is concerned with boundary layer effects on the effective response of fiber-reinforced media. The distribution of the fibres is assumed random. Methodology is presented for obtaining non-local constitutive operators in the vicinity of a boundary and the correctors which provide the stress and strain fields in the constituents. Two types of geometry are considered in the examples: a half-space and a crack in an infinite heterogeneous medium. The influence of non-locality is most pronounced near the tip of a crack, where the stress fields inevitably vary too rapidly for ordinary homogenization to be rigorously applicable. Physically, the most distinctive result is that the stress in a fibre close to a crack tip may be elevated very substantially above the value that would be formally estimated by ordinary homogenization and the associated local corrector.

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Interfacial Microstructurally Induced Failure Modes

Mohammed Zikry* Waeil Ashmawi*
Professor Doctor

Computational schemes have been developed to characterize material failure on the dominant physical scale needed for the accurate prediction of physical mechanisms that control failure initiation, growth, and coalescence. Dislocation-density transmission and blockage interfacial conditions and local stress fields have been obtained for grain-boundary distributions associated with random and tilt orientations. These evolving local stress fields are used as failure criteria to track the initiation, evolution, and interaction of voids. The interrelated effects of grain boundary orientation, dislocation density pile-ups and evolution, geometrical and thermal softening, void distribution and geometry, and hydrostatic stresses on failure paths in cubic crystalline aggregates have been studied.

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Continuum and Atomistic Studies of Intersonic Crack Propagation

Y.Huang*

Professor

Nanotechnology has been identified as a technological area that will have major impact on our life in the 21st century. Research on nanoscale science, engineering and technology (NSET) has attracted scientists and engineers from many fields but few from mechanical engineering. It is commonly believed that the conventional continuum theories are not applicable at the nanoscale (1 to 100 nanometers) such that one has to rely on atomistic studies in NSET research.

Mechanisms of intersonic crack propagation along a weak interface are studied by both molecular dynamics and continuum elastodynamics methods. Part of the objective is to test if continuum theory can accurately predict the critical time and length scales observed in molecular dynamics (MD) simulations. To facilitate the continuum-atomistic linkage, the problem is selected such that a block of linearly isotropic, plane-stress elastic solid consisting of a two-dimensional triangular atomic lattice with pair interatomic potential is loaded by constant shear velocities along the boundary. A pre-existing notch is introduced to represent an initial crack which starts to grow at a critical time after the loading process begins. After propagating at the Rayleigh wave speed for a short time period, an intersonic daughter crack is nucleated at a distance ahead of the mother crack and the daughter crack propagates at the longitudinal wave speed. The challenge here is to test if a continuum elastodynamics analysis of the same problem can correctly predict the length and time scales observed in the MD simulations. Material properties such as elastic constants, fracture surface energy and cohesive strength are determined from the interatomic potential. Based on the Griffith and cohesive strength criteria, it is shown that the predictions based on the continuum analysis agree remarkably well with the MD simulation results.

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Micromechanics-based Continuum Model for Evaluation of Change in Permeability of Discontinuous Rock Due to Excavation of Nuclear Waste Disposal Tunnel

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Professor

Junya Inoue*
Assistant Professor

Hyungmok Kim*
Researcher

Hidenori Yoshida*
Associate Professor

Geological disposal of a high-level nuclear waste in deep underground rock mass has been greatly concerned with the hydraulic characteristics of the jointed rock mass, since groundwater flow is regarded as the only and the most likely means by which radionuclides are transported into our human environments. As intact rock blocks are almost impermeable due to its extremely low permeability, the groundwater flow in the jointed rock mass mainly occurs through discrete joints.

The flow in single rock joint takes place through the connected void space between two rough surfaces of joints, which is usually termed as aperture. The aperture distribution can be significantly changed due to the deformation of joints. In this study, the flow characteristics of single joints and their variation due to the joint deformation were examined through combined deformation-flow analysis in the single joint. The aperture distribution was obtained by the deformation analysis adopting the joint elements, which are suitably defined for the simulation of characteristic normal stress-closure behavior. Using the obtained aperture distribution as an input, the flow characteristics in the single joints were investigated by solving the Reynolds equation numerically.

The Micromechanics Based Continuum (MBC) model was used for the excavation analysis and discrete network model of FracMan/Mafic was selected for the flow analysis in the jointed rock mass. The connection between these two analyses was accomplished by separate module implemented into the FracMan/Mafic. The results demonstrated that the permeability of jointed rock mass can be either increased or decreased due to the excavation, and the tendency was different by the location around the excavation. In particular, the increment in permeability and the reduction of particle travel time in the flow along the tunnel axis were remarkable, when the excavation was created in the jointed rock mass containing two joint sets whose strikes were parallel to the tunnel. Furthermore, considering the anisotropy in transmissivity, the changes could be highly significant.

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Asymptotic Models of Vibration of Elastic Structures in an Electro-Magnetic Field

Alexander Movchan*

Professor

The talk presents results of the recent work concerning interaction between elastic and electro-magnetic fields for vibrating elastic structures. First, we consider a doubly periodic structure of circular dielectric inclusions and develop a regular perturbation algorithm for analysis of photonic-band diagrams; a multi-pole method is used to obtain the dispersion equation and photonic-band diagrams for an array of circular inclusions (unperturbed problem), and the perturbation algorithm provides correction terms associated with the change of shape of inclusions. The second part of the talk includes an asymptotic analysis of attenuation of elastic vibrations of a thin-walled conducting elastic structure placed in a magnetic field, with the applications to the design of filters of elastic waves.

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Constitutive Modeling of Strain-Hardening Hyperelastic Materials

Cornelius O. Horgan* Giuseppe Saccomandi†
Wills Johnson Professor Professor

Constitutive models for incompressible isotropic hyperelastic materials that reflect limiting chain extensibility at the molecular level have been the subject of much recent attention. Such models can account for strain-hardening at large strains, in contrast with classical models such as the neo-Hookean or Mooney-Rivlin models. The new models play a crucial role in current research on the thermomechanics of rubber and the biomechanics of soft tissues. A particularly tractable model is the Gent material, a generalized neo-Hookean model involving a logarithm of the first invariant of the Cauchy-Green strain tensor. This model was proposed by Alan Gent (1996) and gives theoretical predictions similar to the more complicated Arruda-Boyce (1993) eight chain model. In this lecture, we first present an outline of the physical background for such models. Then we consider the solution of some fundamental boundary-value problems of elastostatics for the Gent material. The problems first treated are those of torsion, axial and azimuthal shear. The governing equilibrium equations are nonlinear ordinary differential equations which allow for an explicit analytic solution. The effects of strain-hardening in these shearing problems are thus readily analysed. We then consider the general problem of finite anti-plane shear deformations for the Gent material and give explicitly the governing second-order quasilinear partial differential equation that arises. The anti-plane shear problem for a traction -free crack subject to remotely applied simple shear loading is then investigated. The stress fields near the crack tip for this material are obtained. It is found that the crack-tip stress fields are bounded, in contrast to results for other strain-hardening constitutive models, such as the Knowles' power-law. Thus, the constraint of limiting chain extensibility, in the case of the Gent material, is seen to prevent the development of crack-tip singularities.

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Strain Localization Estimate in Plane Strain by Non-coaxial Plasticity with Double Slip System

Tetsuo Iwakuma*

Professor

A non-coaxial elasto-plastic constitutive relation with the double slip mechanism is applied to predict localization of deformation under the spread foundations and in the sedimentary layer above active faults.

In our phenomenological constitutive model, the total deformation rate tensor is given as

$$d_{ij} = d^e_{ij} + d^p_{ij} + d^m_{ij}.$$

where the first term is the elastic part. The second term refers to the plastic part including a non-coaxial plasticity as

$$\left\{ \overset{\nabla}{\sigma}'_{ij} - \frac{1}{2\overline{\sigma}^2} \sigma'_{kl} \overset{\nabla}{\sigma}_{kl} \sigma'_{ij} \right\}$$

where $\overset{\nabla}{\sigma}'_{kl}$ is the Jaumann rate of deviatoric component of the Cauchy stress, and $\overline{\sigma}$ stands for the effective stress. The third term of the deformation rate tensor is called here the second inelastic mechanism by the double slip on micro-sliding planes with their normal vector $\vec{n}$, and is activated only when

$$\det |n_i F_{ijkl} n_l| = 0; \quad n_k n_k = 1$$

is satisfied, where F_{ijkl} is a modulus tensor between the nominal stress rate and the velocity gradient.

Introduction of this second inelastic mechanism, double sliding, solves to some extent one of the difficulties, such as mesh dependency in the FEM numerical calculations. Emphasis is put on the effect of non-symmetry of loading and the corresponding development pattern of localized deformation. Obtained load-indentation relations become very close to the experimental observations. The pattern of localization is a circular sliding right under the foundation when the eccentricity of loading is large. When the eccentricity is small, two pairs of circular slidings develop in our numerical calculation, which has been also reported in experiments by other researchers. As another example of application of this constitutive model, the ground motion right above an active fault is examined, where a dual development of shear bands is observed.

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Modeling Damage with Shear Bands and Voids in Metals

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Researcher Researcher Professor Graduate Student

An approach for modeling impact damage in metals, based on physical modeling of adiabatic shear bands and void growth, is presented. Scaling laws for damage from adiabatic shear bands have been developed over the past decade following detailed examination of the thermomechanical processes (1). Recently these laws have been adapted for efficient use in large scale computations and show great promise for capturing the essential aspects of diverse experiments ranging from laboratory scale to full scale ballistic impacts (2). A similar approach for ductile void growth and spall has also been initiated (3). A careful analysis of these physical processes has revealed many new and interesting features, which we intend to capture for large scale computations through scaling laws, as well. This approach is expected to lead to damage and failure models that are based on the essence of the physics, rather than on fitting of phenomenological models to large data bases. An added virtue is that it tends to place a premium on accurate measurement and modeling of homogeneous processes, rather than on failure as a separate phenomenon. Finally, the approach also has implications for design and interpretation of experiments.

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Ductile Fracture: Modeling, Simulation, and Experiments

Mark M. Rashid*

Associate Professor

Physically realistic modeling and simulation of ductile fracture processes engenders a range of theoretical and computational challenges. An overview is given of an ongoing research program devoted to the development of practical engineering simulation tools for ductile fracture. The central modeling concept is the "Exclusion Region" theory of fracture, which represents a general theoretical framework for material separation capable of accommodating complex geometry, curvilinear crack extension, and arbitrary bulk material response. The companion computational platform contains a number of novel features, including a "moving mesh patch" finite element overlay which automatically accommodates an extending crack without the need for traditional remeshing. Other advanced features include a material-state-remapping algorithm based on variational enforcement of equality across mesh definitions, and an extremely robust nonlinear solution control algorithm that simultaneously enforces equilibrium and the fracture criterion. Calibration studies have been undertaken with an aluminum alloy and with Inconel 718 thus far. Selected results from these studies will be presented.

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Characterization of Ductile and Brittle Modes of Material Removal Using Single-Grit Scratching

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Professor

Josh E. Loukus*
Visting Assistant Professor

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A generalized approach that couples material deformation modes to data dependant systems (DDS) theory is presented to characterize and quantify the ductile and brittle modes of deformation in materials. The objective is to present, in simple terms, the connection between a deformation mode, the induced topological features and their graphical representation. The concept will be illustrated on typical ductile and brittle materials using two simple and commonly used experiments, namely, normal indentation and single-grit scratching experiments. In each of these situations, the experimentally induced indentation or scratch groove on a specimen will be microscopically analyzed initially and later a three dimensional laser scan of the entire deformed region will be obtained using a laser profilometer. A typical depth profile (at the center of the deformed region) in each of these scans or the associated measured force data will then be analyzed using the DDS approach to extract the frequency components which will be correlated to a specific deformation mode in metals and ceramics. The spread of the components of the frequency spectrum are then used to assess the extent of ductility or brittleness associated with each material or the deformation mode. Finally, the above approach will be validated by conducting experiments on a single material that exhibits both ductile and brittle modes of material removal when the process parameters are changed during the single-grit scratch experiments. Based on the above analysis, a 'brittleness measure' that quantifies the susceptibility for cracking in brittle materials is also developed. The implications of these results for the desired ductile or brittle mode of material removal through appropriate process parameter selection and control during a manufacturing process are discussed.

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Elasticity, Plasticity and Fracture of Thin Films and MEMS Materials : Size Effects in Submicron Gold Films

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Thin films and other small-scale specimens are often found to support significantly larger stresses over their bulk counterparts. This behavior cannot be described by traditional bulk scaling laws and occurs when the specimen dimensions or its microstructure features approach the length scale of the deformation process. The onset of plastic deformation depends strongly on the ability of dislocations to move under an induced stress. The ease of their movement can be hindered by any number of obstacles such as grain boundaries, precipitates, surfaces, etc. When sufficiently small, specimen size begins to govern plastic behavior by creating additional geometrical constraints and surface effects. Other effects that specimen size can have on plastic deformation involve microstructural features associated to film deposition. This includes grain size, morphology, and crystallographic texture, all of which play a role in macroscopic behavior.

The Membrane Deflection Experiment developed by Espinosa and co-workers is used to examine specimen size effects on freestanding thin film gold membranes. It is the first micro-scale testing scheme where the loading procedure is straightforward and accomplished in a highly sensitive manner while preserving the independent measurement of stress and strain. Stress-strain curves will be presented for films 0.3, 0.5 and 1.0 micron thick including membrane widths of 2.5, 5.0, 10.0 and 20.0 micron for each thickness. Several size effects on the mechanical properties were observed including yield stress variations with membrane width and film thickness in pure tension. It was observed that thickness plays a dominant role in deformation behavior of the membranes. A major transition in the material inelastic response occurs when thickness was changed from 1.0 to 0.5 micron. In this transition, the yield stress more than doubled with the 0.5 micron thick specimen exhibiting a more brittle-like failure and the 1.0 micron thick specimen exhibiting a strain softening behavior. SEM images revealed that the number of grains through the thickness essentially halved, from approximately 4 to 2, as thickness decreased. It is believed that this feature limits the number of dislocation sources and active slip systems; hence, other deformation modes such as grain boundary shearing accompanied by diffusion become dominant.

The size effects here reported are the first of their kind in the sense that the measurements were performed under macroscopic homogeneous axial deformation, i.e., in the absence of deformation gradients, in contrast to nanoindentation, beam deflection, and torsion, where deformation gradients occur.

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Inversion of Stress Tensor Using Integrated Photoelasticity

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A new method for non-destructive measurement of an arbitrary 3D stress state using the integrated photoelasticity (Ramesh, 2000) has been developed. Unlike ordinary photoelastic experiments, this method inputs light to an object consisting of a photoelastic material in various directions and obtains images which do not have clear fringe patterns. The 3D stress state within the object is reconstructed by applying computer-tomography techniques to the images. The key issue is the formulation of this inverse problem, since the relation between the 3D stress state and the image is highly non-linear. Taking advantage of the concept of the equivalent inclusion method, the authors succeed to linearize the inverse problem for sufficiently small change in the 3D stress state when the initial state is known (Oguni *et. al*, 2002). Numerical simulation is carried out to verify the validity of the proposed method. It is shown that the non-destructive measurement of the 3D stress state is possible if sufficiently many photoelastic images are taken and images are discretized with high spatial resolution and accuracy.

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Stress Analysis of an Undulated Plate by the Combined First Order Perturbation and Alternating Method

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Structural failures often start from irregular surfaces caused by imperfection due to welding process or corrosion during their service lives. Although numerical methods such as the finite-element method are used for stress analyses, these methods are usually very tedious and time-consuming to calculate the stress distribution near the irregular surface because of the considerably different length scales involved in the problem, i.e. the so-called multi-scale problem. In order to overcome this difficulty, a semi-analytical approach based on the combined first order perturbation and alternating method is proposed in this paper, where attention is focused on the stress analysis of plates of finite thickness with undulating surfaces. Stress concentration at slightly undulating surfaces had been investigated by Gao (1991) using the first order perturbation method, in which undulating surfaces are perturbed from a reference state which is perfectly flat. He applied the method to a half-plane problem in two-dimensions and half-space problem in three-dimensions. Later, a second order perturbation method is applied to two-dimensional problems by Sumi (1995) for the accurate determination of stress gradient and stress distribution in stress concentrated regions. In the present paper a new combined first order perturbation and alternating method is proposed for the analysis of stress concentration in a plate with slightly undulating surfaces, where the perturbation method is applied to satisfy the boundary conditions due to undulating surfaces, while the Schwartz-Neumann alternating method is used to take account of the effect of the back surface, respectively. It is interesting to note that the stress caused by an arbitrarily undulating surface may be approximated by the linear superposition of those arising from regular sinusoidal surfaces having arbitrary wave length and wave direction subjected to in-plane tension-compression and shear because of the linearity of the response with regard to the perturbed surface geometry. This means that we only need the first-order solutions of two-dimensional sinusoidal surfaces subjected to in-plane tension and anti-plane shear as the fundamental solutions in order to solve a problem having arbitrary three-dimensional surfaces. The solution accuracy of the proposed method is examined by comparing the present results with finite-element solutions, and illustrative examples are also given for the stress analysis of corroded plates having slightly wavy random surfaces.

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Bounding the Stress-Strain Response of a Nonlinear Composite

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Professor

The usual approach for obtaining bounds on the response of a composite (linear or nonlinear) is to formulate a principle of "minimum energy" type, and to deduce bounds on the effective potential. For linear media (also for pure power-law media), bounds on the potential imply corresponding bounds on stress-strain behaviour. For more general nonlinear media, however, bounds on the potential do not provide any rigorous information about the stress-strain response, which is given in terms of the gradient of the potential. This work builds on an idea of G W Milton, in providing bounds of Hashin-Shtrikman type directly on the set in strain space, within which the effective stresses and associated strains must lie. This is done by bounding a "potential" in stress-strain space, which comprises the characteristic function of the set within which the stress-strain relation is obeyed. This characteristic function is zero on the stress-strain relation and infinity otherwise, so any positive lower bound on the effective potential implies that the stress-strain relation must be violated somewhere. The innovation is the use of machinery of Hashin-Shtrikman type, to obtain such bounds. An equivalence between results obtained by the new method and those obtained by bounding the energy is demonstrated in the case of linear response. Nonlinear examples show that effective stress-strain curves obtained by differentiating the energy bound coincide with the new bounds in some simple cases but not generally.

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Quantum/Atomistic/Continuum Coupling in Materials Simulation

(Symposium No. 16)

Organizers:
Harley Johnson, University of Illinois – Urbana-Champaign
William A. Curtin, Brown University

Connecting Atomistics to Continuum Elasticity: Modeling Vacancies in Stillinger-Weber Silicon

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Vacancies in silicon undergo an elastic relaxation that contributes to the formation energy of the defect. This elastic relaxation can also couple the defect energy to an externally applied elastic field. Understanding this coupling is important for modeling the effects of stress on microstructure and predicting transport properties in the crystal. We have performed molecular dynamics (MD) calculations of the relaxation and coupling in Stillinger-Weber silicon. Comparisons were made between these atomistic results and Green's function solutions of the elastic relaxation around a generalized force dipole. In these comparisons the boundary conditions of the elasticity calculation were extracted directly from the MD simulation rather than by fitting the long-range elastic behavior. The formation energy and symmetry of the defect can change due to hydrostatic and anisotropic loadings. We will discuss the extent to which the defect itself can be modeled as isotropic and under what conditions it undergoes a change in symmetry. The elastic displacement field predicted by continuum mechanics methods is then compared directly to the atomistic results. The effect of temperature on the defect symmetry and formation energy will also be discussed.

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Atomistic and Continuum Analysis of Residual Stress Effects in an Ion-Beam Machined Thin Film MEMS Structure

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A combined molecular dynamics and continuum mechanics approach is used to study the process by which ion-beam damage leads to residual stress evolution and curvature change in a thin film MEMS structure. The analysis helps to explain a newly developed experimental process that relies on amorphization stress at the surface of a free standing thin film to reduce the curvature of the structure. [1] At the continuum level, the model is based on the familiar approach in thin film mechanics that relates in-plane mismatch stress to wafer curvature. [2] Here the entire structure, which is a fully functional MEMS device used for optical applications, is only several microns thick. Since the mismatch stress distribution is nonuniform in this case, the continuum analysis goes beyond the standard Stoneys equation approach. Furthermore, the mismatch stress field itself is not well understood, so molecular dynamics simulations are first used to model the process by which the ion-beam induces damage and stress near the surface of the film. The ion bombardment process is similar to ion implantation methods for doping semiconductor thin films, [3] but has considerably lower incident ion energies. The molecular dynamics simulations consist of modeling the transient process by which individual incident ions penetrate a crystalline Silicon thin film and create defects and damage. A statistical analysis of the resulting equilibrium microstructure leads to an estimate of the average through thickness residual stress distribution on a cross section of ion-machined thin film. This stress distribution is then used in the continuum model to compute the resulting curvature change in the structure. Curvature change estimates are in reasonable agreement with experimentally observed values.

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Dynamically Equivalent Continuum Interpretation of Discrete Molecular Behavior at Arbitrary Scales

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The continuum interpretation of results of molecular theories is an important task in the scale-up of nanoscale characterizations of material behavior. Issues involved include continuum stress interpretation of discrete atomic force fields at nanoscales, body and surface forces due to the effects of nonlocal interactions, and discreteness- and nonlocality-induced length scales. Such effects must be captured and quantified when a transition is made from discrete molecular dynamics to continuum mechanics. Despite their different discrete and continuous perspectives, these atomistic and continuum theories are based on the same fundamental laws, including Newtons laws of motion, conservation of energy, and conservation of mass. These fundamental laws provide a basis for interpretations of the results of one description in the context of the other. An equivalent continuum is defined for dynamically deforming atomistic particle systems treated with concepts of molecular dynamics. The equivalence of the continuum to the discrete atomic systems includes (1) preservation of linear and angular momenta, (2) conservation of internal, external, and inertial work rates, (3) conservation of mass, and (4) preservation of kinetic energy. Construction of the continuum fields follows a process in reverse to finite element discretization. The momentum- and work-equivalence is achieved by virtue of the principle of virtual work for fully dynamic conditions. This equivalence holds for the entire system and for volume elements defined by any subset of particles in the system; therefore, averaging and characterization across different length scales are possible and size-scale effects can be explicitly analyzed. The framework of analysis provides explicit account of arbitrary atom arrangement, admitting applications to both crystalline and amorphous structures. The analysis also applies to both homogeneous materials with identical atoms and heterogeneous materials with dissimilar atoms. For nonpolar atomic systems with only central interatomic forces, the fields of couple stress, body moment, and surface moment vanish. This result demonstrates that, at the atomic level, the origination of couple stress requires interatomic moment interaction.

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Mechanics of Carbon Nanotubes: A Continuum Analysis Incorporating the Interatomic Potentials

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Carbon nanotubes show great promise for applications ranging from nanocomposites, nanoelectronic components, nanosensors, to nanoscale mechanical probes. These materials exhibit very attractive mechanical properties with extraordinarily high stiffness and strength, and are of great interest to researchers from both atomistic and continuum points of view. The studies on carbon nanotubes, however, have all been limited to the atomistic simulations since the single-wall carbon nano-tubes contain only a layer of carbon atoms in the wall thickness direction. It is commonly believed that the continuum mechanics theories are not applicable at this level.

We have developed a continuum theory for single-wall carbon nanotubes by incorporating the interatomic potential between carbon atoms into a continuum constitutive model for the nanotube wall. Once the interatomic potential is known, no fitting parameters are introduced in the continuum analysis. We have studied several examples, including the relation between energy and tube radius prior to deformation, elastic modulus, fracture nucleation, defect formation in carbon nanotubes, as well as the change of electrical property due to mechanical deformation. We have also included the temperature effect in our continuum analysis of carbon nanotubes, and studied the thermal expansion coefficient of carbon nanotubes. Our continuum analyses agree very well with the atomistic studies without any parameter fitting.

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Nonlocal Separation Constitutive Laws for Interfaces Informed by Nano-Scale Simulations

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By incorporating nano-scale fracture characterization using molecular dynamics (MD) simulations based on Embedded Atom Method (EAM) potentials [1,2], an integrated framework is developed to characterize fracture through continuum interface separation constitutive laws that are atomistically motivated. Such constitutive laws may ultimately be implemented in robust analyses of distributed fracture in complex microstructures using the Cohesive Finite Element Method (CFEM) [3]. These laws are distinguished from previous continuum models in that discrete atomistics are used to model the nano-scale effects, such as the nature of atomic structure and imperfections for the initiation and propagation of cracks.

Incorporation of molecular dynamics with the CFEM fracture model to account for fracture at various hierarchical levels is accomplished by considering the normalization of tangential and normal interface separation components by path-history dependent parameters which depend on a set of material interface attributes. This set of interface attributes is comprised of interface geometry, defect density into the bulk, and includes a measure of damage (broken bonds) along the interface. Geometric attributes include length, width, and depth of a specimen relative to its inter-atomic spacing, along with the coherency of the interface between two materials. The role of dislocations is highlighted in a series of simulations for Cu-Cu interfaces involving both normal and shear separation, as well as sequences of normal-shear and shear-normal deformation relative to the interface. The evolution of damage in the separation process zone is considered as a function of non-equilibrium loading path. These results will be presented, along with a framework for informing continuum models with nano-scale fracture/dislocation phenomena.

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Evolution of the Dislocation Core Structure During Dislocation Glide in an FCC Lattice

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A dislocation core model is developed in terms of a singular decomposition of the elastic field surrounding the dislocation in a power series of 1/rn. The decomposition is a Laurent expansion beginning with the term corresponding to the Somigliana dislocation and continuing with a series of dipoles and multipoles. The analysis is performed for both edge and screw dislocations located in a model Morse material. The field surrounding the dislocation is derived by atomistic simulations. The coefficients of the series expansion are determined from the elastic field using path independent interaction integrals. The decomposition is a signature of a given dislocation type. When loaded by a shear stress smaller than the Peierls stress, the core distorts. The distortion up to the instability (Peierls stress) is monitored based on the variation of the coefficients. The implications for energy dissipation by phonon emission are discussed.

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Dislocation Motion in Al-Mg: Computer Simulations of Solid Solution Hardening

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Solid solution hardening is an important metallurgical tool, and has been the subject of a number of theoretical and computational studies. When the impurity diffusion is fast compared to the dislocation velocity, a Cottrell atmosphere can form about the dislocation and move with it [1]. Much of the continuum modeling has focused on this case [1-3]. If the diffusion is much slower than the dislocation motion the impurities cannot keep up with the dislocation, and the solute drag on the dislocation is smaller. While this case has been studied less intensively, two-dimensional continuum simulations suggest that the dislocation mobility can still be substantially reduced compared to the pure metal [3].

Because dislocations are not perfectly straight, and because the distribution of impurity atoms in three dimension will affect the shape of the dislocation, fully 3d analysis or simulations are needed to fully investigate these issues. This work reports on simulations in the limit in which the solute atoms are randomly distributed, and cannot diffuse on the time scale of the dislocation motion. Using molecular dynamics and classical potentials, the motion of a single dislocation is simulated under both conditions of higher applied stress where the dislocation moves fairly steadily and lower applied stress where the dislocation can be pinned by particular impurity configurations.

For the case of continuous motion, dislocation velocities as a function temperature and stress are obtained directly from the molecular dynamics simulations. Even in this case, where no pinning takes place, the dislocation mobility is significantly reduced in comparison to pure Al. For the case where the stress is low enough that the dislocation becomes pinned by a particular solute configuration, it is useful to focus on the effective energy landscape in which the dislocation moves. While there is qualitative agreement with the expectations of continuum elasticity theory, atomistic effects resulting from local relaxation of the dislocation core are important.

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A Stress-Gradient Based Criterion for Dislocation Nucleation in Crystals: Theory and Simulation

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A central issue in a full understanding of the basic physics of the plasticity and strength of crystalline solids is a theory of dislocation nucleation. Specifically, it is of interest to have a criterion that can predict what mechanical conditions (deformation state) will lead to the homogeneous nucleation of a dislocation. A natural assumption is that the nucleation of dislocations is governed by a critical stress criterion, whereby new defects will form when a certain stress level is achieved at a point in the crystal. In this work, we demonstrate that a stress-based criterion is incorrect, and present a new criterion based on the gradients of the stress tensor that accurately predicts dislocation nucleation. The nucleation criterion that we present is derived from a continuum mechanics-based theory of continuously distributed dislocations, and reduces to a scalar function involving the curl of the stress tensor and the geometry of the nucleated dislocation. In order to test the predictive capabilities of the criterion, we present a series of atomistic simulations of dislocation nucleation, including nano-indentation by a spherical indenter and uniaxial stretching of a crystal containing an atomic-scale void. Through detailed analysis of the atomic level stresses prior to nucleation, we show that the new criterion exactly predicts the location and type of the nucleated defect in each case. Further, we demonstrate that the widely used assumption of a critical nucleation stress does not accurately predict the results of these same simulations. The simulations are facilitated by using the recently developed CADD (coupled atomistics and discrete dislocations) technique of Shilkrot, Miller and Curtin [1]. This method directly couples an atomistic region to a linear elastic continuum. Its main advantage over other similar coupling techniques is its ability to support discrete dislocations, as elastic defects, in the continuum region. As well, the method automatically detects dislocations which form in the atomistic region and move to the continuum region, correctly 'converting' from the atomistic to the continuum description of the defect. In this study, the CADD method allows for larger systems than direct atomistics, as well as providing a convenient tool to detect and identify dislocations as they nucleate.

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Phase Field Modelling of the Portevin-Le Chatelier Effect from the Dynamic Drag of Solute Atmosphere

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A solute atmosphere is typically formed around a moving dislocation in a solid solution at the range of temperature where the diffusion of solute atoms is comparable with the dislocation velocity. The dragging stress on the dislocation motion by this atmosphere is important for the mechanical properties of alloys. In present talk, the dynamic interactions between solute diffusion and dislocation motion under applied stresses are studied in three dimensions, using a phase-field models for integrating phase and defect microstructures. It takes into account both the chemical interaction between solutes and the elastic interaction among solutes, dislocation and other crystalline defects. It allows arbitrary distribution of composition and dislocations in three dimensions and does not explicitly track the positions of dislocations and solute atoms during dislocation and solute profile evolution. The focus of this talk will be on the Poetevin-Le Chatelier Effect of solute atmosphere. The concurrent motion of dislocation and solute atom cloud and breakaway of a dislocation from the solute atom cloud are analyzed based on the dislocation velocity, the effective stress, and the solute segregation profile around the moving dislocation. The segregation process of solutes around a moving dislocation, the dependence of steady-state and non-steady state solute distributions on the chemical interactions among solute atoms, the temperature, and the dislocation velocity are systematically studied.

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Multiscale Modeling of Plasticity in Dynamic Fracture of Ductile Metals

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We study the nucleation and growth of voids associated with dynamic fracture in ductile metals, with an emphasis on the concomitant plastic deformation and how information obtained at the atomistic level can be linked into dislocation dynamics simulation. The nanoscopic mechanisms of this high strain-rate plasticity have not been studied previously in detail. Large-scale molecular dynamics (MD) simulations have been used to characterize the dislocation structure and evolution during void growth in single crystal and polycrystal copper. The MD methodology for void growth developed by Belak [1] has been extended recently to allow on-the-fly characterization of dislocation activity at finite temperature in the plastic zone surrounding voids growing under tensile loading (cf. [2]). In a typical simulation, the initial configuration includes a pre-existing void or weakly bound inclusion. This system is brought to thermal equilibrium, and then a dilatational strain is applied that induces void growth. The resulting dislocation activity serves to transfer material away from the void, and is intimately associated with void growth. The role of dislocation loops has been studied in detail. We have further identified the character of the most numerous dislocations and their associated glide planes. This information is used to formulate a dislocation dynamics model of void growth for the single crystal case. Recently these techniques have been used to investigate the effect of strain triaxiality.

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A Superposition Framework for Discrete Dislocation Plasticity

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A superposition technique is introduced which allows the straightforward application of discrete dislocation (DD) plasticity to a wide range of thermo-mechanical problems with reduced computational effort. For many bimaterial systems (ie thin metal film on a large ceramic substrate) only part of the structure is modelled as containing dislocations. In these and other non-symmetric problems, existing DD machinery becomes computationally expensive as the number of dislocations and/or amount of material exterior to the dislocation region increases. Here, such problems are solved by superposition of two subproblems. The first subproblem is a dislocation-free model of the entire structure, subject to the desired loading and boundary conditions. The second subproblem is a DD model of that part of the structure where dislocation phenomena are permitted, subjected to either zero traction or zero displacement boundary conditions. The two subproblems are not independent: the stress field of the dislocation-free subproblem drives evolution of the dislocations in the DD subproblem while the negative of the boundary tractions arising from the DD subproblem are applied as body forces on the corresponding boundary of the dislocation-free subproblem. The effect of the applied loading on the DD subproblem enters only through the stress field of the dislocation-free subproblem. In this way the DD calculation is completely general, and does not depend on the type of applied loading or the extent of material external to the dislocation region. The method is used to examine crack growth along an elastic-plastic/elastic bimaterial interface.

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Couple Stresses in Crystalline Solids: Origins from Plastic Slip Gradients, Dislocation Core Distortions, and Three-Body Interatomic Potentials

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In the presence of plastic slip gradients, compatibility requires gradients in elastic lattice rotation and stretch tensors. For a crystal lattice, the gradient in elastic rotation is related to the change in bond angle at the core of dislocations. These are the so-called 'geometrically-necessary dislocations'. The corresponding strain energy is represented by three-body interatomic potentials. A couple stress tensor arises in the continuum limit. The resulting stress and couple stress, strain and strain gradients satisfy a balance law and boundary conditions originally due to Toupin. Toupin's theory has been extended in this work to incorporate constitutive relations for the stress and couple stress under multiplicative elastoplasticity. This higher-order continuum theory is exploited to solve a boundary value problem of relevance to single crystal and polycrystalline nano-devices. The important implication is derived, that the assumed deformation mechanism makes nanostructures significantly more compliant in bending-dominated situations.

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Quantum-Atomistic Study of Interdiffusion in Si/Si1-xGex Multilayer Structures

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Understanding interdiffusion in SiGe systems is important from both a technological and a scientific point of view. Technologically, SiGe is becoming important for applications in high frequency & low power devices. Scientifically, SiGe is a rather clean system for a theoretical study of diffusion in random alloys as it is free from complications associated with charge states and such as would be present in the case of other non-isovalent dopants like Boron or Phosphorous. Experimentally, Si/Si1-xGex multilayers have been observed(1,2) to exhibit a time dependent interdiffusivity. It is the purpose of this work to determine, from first principles, the reason for this time dependence. Based on our energetics calculations of vacancies in Si1-xGex, we have hypothesized that a probable reason for the time dependent interdiffusivity is the Ge concentration dependent vacancy formation energy arising out of Ge V attraction. In order to test our hypothesis, we have compiled a first principles rate database for vacancy diffusion in various environments. Using this database, we have performed a kinetic Monte Carlo simulation of the interdiffusion process. Presently, we have performed such a simulation with a constant vacancy concentration and we obtain a constant (time independent) interdiffusivity. We are working on performing a similar simulation with a varying vacancy concentration. We hope to be able to reproduce the experimentally observed time dependent interdiffusivity.

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Flexible First-Principles Boundary Conditions: Simulating Isolated Dislocations in Metals

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Research Scientist

First principles (FP) methods (e.g., electronic structure methods based on Density Functional Theory) provide a direct way of sampling how changes in chemistry influence materials properties. Recent improvements in numerical stability and parallel processing make FP simulations of several hundred atoms fairly routine. However, these are still very small simulation cells given the complexity of real alloy systems and the defects they contain. We offer a strategy for modeling defects in metals using informed boundary conditions, which are, derived from FP reference calculations. A flexible boundary condition method has been developed which can contain extended defects in very small simulation cells. Here the local strain field is self-consistently coupled to the long range elastic field using a lattice Greens Function method. This reduces the mesoscopic atomistic calculation to one only involving only the degrees of freedom near the defect center. As proof of concept FP methods have been used to evaluate the core structure and Peierls stress of isolated dislocations in BCC Mo, Ta and L10 TiAl. Predicted non-Schmid behavior in the BCC metals is consistent with experimental measurements. Also, the local strain field of the ordinary screw dislocation in TiAl gives insight as to the nature of the anomalous yield stress observed at high temperatures. These methods offer a clear path for directly evaluating solute-dislocation interactions and predicting solid solution strengthening.

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From Quantum-Mechanics to Fracture: Atomistics Multiscale Simulations of Silicon

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Research Physicist

Silicon, long studied as a model system for the transition between brittle and ductile fracture, has proven to be difficult to simulate because of the failure of popular empirical potentials such as Stillinger-Weber and EDIP to describe even the apparently simple brittle regime. We have addressed this problem using an atomistic method with a Green's function based tight binding and an empirical potential coupled together dynamically (GTEC). Results of simulations using this method are in agreement with experimental observations of brittle fracture at the elastic energy threshold for crack propagation (the Griffith criterion). We find that fracture criteria based on energy balance do not explain the difference between the empirical potentials and the GTEC method. We show that a simple quantitative model for the energy barrier to fracture propagation (lattice trapping) correctly predicts the initiation of fracture. Using this model we analyze the length and energy scales that are relevant to brittle fracture.

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Coupled Atomistic and Discrete Dislocation Plasticity

Leonid Shilkrot* W. A. Curtin* Ronald E. Miller†

Research Associate Professor Professor

A computational method for multiscale modeling of plasticity is presented where each dislocation is treated as either an atomistic or continuum entity within a single computational framework that allows the description of each dislocation to change from atomistic to continuum as dictated by local conditions. The method divides space into atomistic and continuum regions that communicate across a coherent boundary, detects dislocations as they approach the boundary, and seamlessly converts them from one description to another. This approach makes it possible to zoom in on the regions of the material where atomistic effects such as large deformations, decohesion, or bond breaking at the tip of a growing crack, play a dominant role, while retaining the information about all other dislocations treated as continuum defects. The coupling between the atomistic and continuum regions of the material is achieved by imposing a set of boundary conditions at the atomistic/continuum interface. The present formulation makes it possible to solve for the elastic field in both the atomistic and continuum region as a minimum of the total energy functional combining the energy of the atomistic region with the energy of the elastic continuum containing discrete dislocations. We validate our approach by presenting simple test problems permitting direct comparison with atomistic simulations. Other possible methods of joining the atomistic and continuum regions of the material are also discussed.

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Multiscale Modeling of Laser Ablation of Organic Materials and Metals

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Assistant Professor

Short-pulse laser irradiation of a solid target can induce a range of non-equilibrium processes in the surface region of the target, from strong overheating and fast melting to an explosive boiling and massive material removal (ablation). Practical applications based on short-pulse laser irradiation include surface processing and microfabrication, laser surgery, and mass spectrometry of large biomolecules. Computational modeling of the laser-induced processes has a potential of making an important contribution to the advancement of the applications. In this presentation, two computational schemes developed for simulation of laser coupling to organic materials and metals are discussed and a multiscale approach that addresses different laser-induced processes with appropriate resolutions and, at the same time, accounts for the interrelations between the processes is presented.

In the multiscale model the initial stage of laser ablation is reproduced by the classical molecular dynamics (MD) method. For organic materials, the breathing sphere model is developed to simulate the primary laser excitations and the vibrational relaxation of excited molecules. For metals, the two temperature model coupled to the atomistic MD model provides an adequate description of the laser light absorption by the conduction band electrons, the energy transfer to the lattice due to the electron-phonon coupling, and the fast electron heat conduction. A combined MD - finite element method approach and a dynamic non-reflecting boundary condition are used to simulate propagation of the laser-induced pressure waves out from the MD computational cell, allowing us to focus our MD computational efforts on the areas where active processes of laser-induced melting/damage/ablation are occurring. The direct simulation Monte Carlo method is used for simulation of the multi-component ablation plume expansion on the time- and length-scales of real experimental configurations. The essence of the computational approach and application of the model to the analysis of different modes of cluster ejection and the resulting cluster size distributions in the ablation plume will be covered in the presentation.

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Simulation Based Control
(Symposium No. 17)

Organizers:
Richard A. Wysk, The Pennsylvania State University
Young-Jun Son, University of Arizona

A Bidding-Based Control Framework for a Random Flexible Manufacturing System with Alternate Routings

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Graduate Student

Can Saygin*
Assistant Professor

This paper presents the results of a simulation study of a random flexible manufacturing system (FMS) that has routing flexibility. The objective of this study is to test the effectiveness of a bidding-based real-time control framework and to explore the impact of part-based autonomous decision making for routing selection. The overall system performance is evaluated based on the amount of deviation between the actual completion times and the due dates.

The control architectures of flexible manufacturing systems have evolved from centralized and hierarchical structures to more distributed structures. Various researchers propose heterarchical architectures, which consist of a number of distributed and autonomous agents that communicate with each other to cooperatively manufacture parts. A widely used scheme for achieving cooperation among these autonomous control entities in heterarchical systems is to use a bidding approach based on the contract net protocol. Various decision-making algorithms are used in bid evaluation varying from simple dispatching rules to complicated mathematical equations. However, the overall system behavior usually cannot be controlled by using only a bidding scheme. A reward mechanism that provides feedback on the success of certain events that occur after the bidding process is essential to avoid myopic decisions. This paper proposes a bidding-based framework that consists of a reward mechanism for real-time FMS control. Parts select the best route by requesting completion time-based bids from the machines along the alternate routes.

A simulation study has been conducted to compare the proposed framework with various dispatching rules. The study presents the conclusions and future research directions to further improve the proposed framework.

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Simulation-based Control for an Automated Workstation

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Amit Pai*
Graduate Student

This presentation describes a schedule-generation approach for control for automated workstations. The class of workstations considered includes multiple processing machines served by a single automated material-handling device. This problem is similar to the traditional job shop problem in which n jobs need to be scheduled on m machines, except that the material handling steps between processing operations must be explicitly considered to facilitate control of the workstation. The inclusion of the material handling operations complicates the general scheduling problem as it introduces both resource and temporal constraints. An existing schedule-generation algorithm has been modified to include material handling operations. The controller carries out a multiple simulation runs using local search in order to select the best schedule.

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Real-time Adaptive Shop Floor Control System: Using Simulation, Dispatching Rules, and Direct Search Algorithm

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Graduate Student Graduate Student

Jayendran Venkateswaran* Young-Jun Son*
Graduate Student Assistant Professor

A shop floor control system, SFCS, performs the decision-supporting, decision-making (task-generating), and execution functions necessary to fill the production orders efficiently. To cope with various dynamic, environmental factors – such as a variety of customer demands, customer-designed products, and shortened product life cycles– the SFCS must be able to perform these functions in real-time. This paper presents a real-time shop floor control methodology which uses simulation, dispatching rules, and direct search algorithm (e.g., scatter search). The work in this paper has been based on the simulation-based control of RapidCIM project (Wysk et al., 1992), where an enhanced discrete event simulation is used as a real-time decision-maker (task generator). The decision-maker in a supervisory controller parses XML-based process plans into a non-linear graph structure and then resolves the AND-nodes and OR-nodes, determining the sequence of tasks and generating the set of messages associated with those tasks. The decision-supporter, when called by the decision-maker, evaluates several set of control rules using a corresponding simulation model, chooses the most promising set of rules using a direct search algorithm given real-time constraints, and provides it for the decision-maker. This paper will discuss the modeling parameters that are significant to the overall performance of the proposed real-time adaptive simulation-based control system. This paper will also present implementation issues, including 1) enhancement of commercial simulation software to handle XML-based alternative routings and 2) integration of Arena real-time simulation with a direct search algorithm in OptQuest. Finally, this paper will present the experimental results of the proposed method for a test flexible manufacturing system.

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Tool Management in Flexible Manufacturing Systems: A Simulation Study

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Graduate Student

Can Saygin*
Assistant Professor

In this paper, a heuristic for tool selection and allocation in flexible manufacturing systems (FMS) with cutting tool alternatives is presented. The heuristic is utilizes on a new metric, which takes tool life and tool size into consideration. The metric is the ratio of tool life (L) over tool size (S), which is referred to as L/S ratio. It gives the virtual life of a cutting tool per slot in the tool magazine. The heuristic is practical for FMS where lead times are low, batch sizes small, and shop floor control functions are automated and highly integrated. The heuristic selects tool types with high L/S ratios by considering the existing tool alternatives for the operations assigned to each machine.

The study also presents a survey of several approaches related to loading and tool allocation problems in FMS and aims at highlighting the importance of tooling and the practical aspects of tool-oriented decision making. The lack of practical aspects in the existing models is also underlined.

A simulation study has been conducted to compare the effectiveness of the proposed heuristic. The proposed approach has been benchmarked against various tool selection and allocation approaches. The study presents the conclusions and future research directions to further improve the proposed framework.

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Student Paper Competition

(Symposium No. 18)

Organizers:
William Thompson, Jr., The Pennsylvania State University
Charles E. Bakis, The Pennsylvania State University

Finite Strain Response and Texture Evolution of *alpha*- and *beta*- Crystalline Polypropylene

Wei Xu*
Graduate Student

Ellen M. Arruda†
Associate Professor

An experimental study of the finite strain response and morphological evolution of annealed *alpha* and *beta* crystalline isotactic polypropylene (iPP) was conducted over a range of temperatures (25, 75, 110 and 135 ^{circ}C) using uniaxial compression tests. 69% crystalline *alpha*-iPP specimens and 74% *beta*-iPP specimens were prepared by melt crystallization under identical heat treatment histories. Morphological evolution with inelastic deformation was examined using Differential Scanning Calorimetry (DSC), Wide Angle X-ray Scattering (WAXS) analysis and Scanning Electronic Microscopy (SEM)after unloading from increasing amounts of inelastic deformation. DSC and WAXS investigations of *beta*-iPP revealed a continuous transformation of *beta* crystals to *alpha* crystals with inelastic deformation at room temperature. This transformation was facilitated at higher temperatures. Uniaxial compression results indicate nearly identical macroscopic stress vs. strain behavior for *alpha*-iPP and for *beta*-iPP to true strains in excess of 100% at room temperature despite the different initial morphologies and the *betarightarrowalpha* transformation. At larger compressive strains (>1.2), *beta*-iPP shows more rapid strain hardening. The orientation of crystalline planes during straining differs at room temperature from that at high temperature, indicating a change of slip mechanisms as temperature increases. Also strain-induced crystallization occured at the highest temperature examined in *alpha*-iPP. The *betarightarrowalpha* transformation occurred with no evidence of a mesomorphic phase nor melting. A solid-to-solid mechanism for the *betarightarrowalpha* transformation is proposed based on the propagation of defects and a shear (Martensitic) transformation of the crystal lattice during deformation. This mechanism is supported by SEM observation since epitaxially grown secondary lamellae have not been found in transformation-produced *alpha* crystals, which are typical in melting crytallized *alpha* spherullites.

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Thermodynamic Framework for Coupling of Non-Local Viscoplasticity and Non-Local Anisotropic Viscodamage for Dynamic Localization Problems Using Gradient Theory

Rashid K. Abu Al-Rub* George Z. Voyiadjis*
Doctoral Candidate Boyd Professor

Anthony N. Palazotto†
Professor

This study develops a general consistent and systematic framework for the analysis of heterogeneous media that assesses a strong coupling between viscoplasticity and anisotropic viscodamage for dynamic problems within the framework of thermodynamic laws and gradient theories. Since the material macroscopic thermomechanical response under dynamic loading is governed by different physical mechanisms on the meso- and macroscale levels, the proposed model is introduced with manifold structure accounting for discontinuous fields of dislocation, crack, and void interactions. The gradient theory of rate-independent plasticity and rate-independent damage that incorporates macroscale interstate variables and their higher-order gradients is generalized here for rate-dependent plasticity and rate-dependent damage to properly describe the change in the internal structure and in order to investigate the size effect of statistical inhomogeneity of the evolution-related rate- and temperature dependent materials. The idea of bridging length-scales is made more general and complete by introducing spatial higher-order gradients in the temporal evolution equations of the internal state variables that describe hardening in coupled viscoplasticity and viscodamage models, which are considered here dependent on their local counterparts. The constitutive equations for the damaged material are written according to the principle of strain energy equivalence between the virgin material and the damaged material. Computational issues concerned with the current gradient-dependent formulation of initial-boundary value problems are introduced in a finite element context. A weak (virtual work) formulation of the non-local dynamic viscoplastic and viscodamage conditions is derived, which can serve as a basis for the numerical solution of initial boundary value problems in the sense of finite element method. Explicit expressions for the generalized tangent stiffness matrix and the generalized nodal forces are given.

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Strain Rate Sensitivity of Cymat Aluminum Foam Subject to Uniaxial Compressive Loading

Matthew M. Braun* Kathleen A. Issen†

Undergraduate Student Professor

In recent years the proposed use of lightweight aluminum alloy foam for service in energy absorption roles, such as those of automotive bumpers and packaging materials, has gained momentum. In order to effectively incorporate this material into designs, a full understanding of its mechanical behavior related to energy absorption must be obtained. One such aspect of this behavior is strain rate sensitivity. Previous work conducted under both quasi-static and dynamic test conditions on various types of foam indicates that metallic foams exhibit strain rate dependencies to varying degrees. A general trend in the data suggests that closed cell, cast, and high relative density foams, are the most likely (although not certain) to exhibit a strain rate sensitivity. Our present work focuses on characterizing the strain rate dependence of a specific high relative density, semi-closed cell, cast aluminum alloy foam manufactured by Cymat Inc. Samples were uniaxially compressed to 60% strain at various strain rates over a range of 1e(-5) s(-1) to 1e(-1) s(-1), and load and displacement data gathered. Strain rate influence characteristics (peak stress levels, plateau stress levels, and energy absorption traits) have been quantified from this data, and contrasted with available data for other foams.

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Experimental Analysis of Compaction Band Formation in Aluminum Foam Using Surface Strain Mapping

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Kathleen A. Issen*
Faculty Advisor

Aluminum foam is a lightweight cellular metal suitable for a number of applications including: impact energy absorption, structural damping, and sandwich core fillers. Understanding the mechanical behavior (both elastic and plastic) of this material is key to unlocking its full design potential. In previous works, the existence of macroscopic localized deformation bands orientated perpendicular to the loading axis, compaction bands, have been observed to develop and propagate under quasistatic uniaxial compression loading. However, this phenomenon has yet to be fully documented. The precise onset of compaction band formation is unclear and has typically been described as occurring pre-peak. Therefore our current work focuses on determining the loading conditions and material properties at localization. Digital images were acquired and surface strains maps correlated and analyzed for 55 mm cubic specimens of 15% relative density Cymat semi-closed cell aluminum foam. Axial and lateral strains were extracted from correlated data to determine whether the compaction band forms during the linear, nonlinear, or peak portion of the loading curve. A series of unloading loops were used to extrapolate the elastic and plastic components of strain, Youngs modulus, and Poissons ratio prior to the formation of the compaction band. Discussion of results includes a real time video of specimen deformation, stress strain relations, and surface strain mapping.

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Tissue Engineering and Characterization of Self-Organized Tendon Constructs

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Graduate Student

Robert G. Dennis†
Professor

Karl Grosh*
Professor

Ellen M. Arruda*
Professor

We have created self-assembled collagen-based tendon-like constructs. A parametric study of variables known to influence the behavior of tendon fibroblasts in vitro (substrate, concentration of fetal bovine serum, environment of cell before plating, ascorbic acid concentration) are underway to engineer constructs that more closely mimic tendon physiology and function. The histology and stress-strain response of a variety of engineered tendon constructs will be characterized.

Tendons are essentially parallel fibers of collagen, approximately 70% of the dry weight, interspersed with fibroblasts, both of which are responsible for the development and maintenance of tendon physiology. Our goal is to combine these tendon constructs with self-assembled muscle constructs, termed myooids, which have been developed in our lab via stress-mediated self-organization. Myooids can transmit force spontaneously and upon the application of an electrical stimulus. They display an immature phenotype both morphologically and mechanically however, which hinders their use as a model of in vivo muscle function. It is well known that mechanical stimuli are an important factor in muscle and tendon development and we plan to manipulate this response to facilitate maturation. The creation of tendon constructs was motivated by the need for an anchor that will form a strong interface with muscle that can withstand cyclic mechanical stimuli of physiological intensity, but we do not currently have a suitable anchor for the tendon constructs. While bone would be the ideal material to anchor our tendon constructs, an inert material is preferred for repeatable and biocompatible use. We are currently investigating various methods to properly functionalize porous polyethylene (PE) for use as an anchor such as oxidation by plasma discharge treatment and sulfonation by exposure to concentrated sulfuric acid.

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Conditions for Localized Compaction in High Porosity Sandstone

Vennela Challa*

Student

Compaction bands are a form of localized deformation found in field and laboratory specimens of high porosity rock, consisting of planar zones of pure compressional deformation forming perpendicular to maximum compression. Experimental results indicate that compaction bands and/or shear bands (where the band normal forms a low angle with respect to the direction of maximum compression) occur in high porosity sandstone during a transitional regime where multiple damage mechanisms may be active. A two yield surface constitutive model where the shear surface corresponds to a dilatant frictional mechanism and the cap corresponds to a compactant mechanism, is used to examine localized deformation conditions. While a single yield surface constitutive model predicts shear bands, the two yield surface model predicts both experimentally observed band types for reported values of key parameters. This work extends the predictions of the two yield surface model to further refine the k=0 case. Specifically, if the slope of the mean stress-inelastic volume strain curve, k is approximately zero (corresponding to the characteristic plateau), then only compaction bands are predicted when normality is assumed for the cap. For the deviations from cap normality, low angle shear bands are predicted. The shear band region forms a zone of transition between the compaction bands and dilation bands and the predictions in this region are examined. The theory allows for the formation of shear bands which are observed experimentally. The predictions of the two yield surface model were examined for cases where k was not equal to zero and the results compared with experimental observations. Conditions for compaction band formation are less favorable if k is less than or equal to 0 or k is very small as compared to G (the shear modulus for elastic unloading), since the value of the hardening modulus required for localization becomes negative for cap normality. Conditions for shear band formation are more favorable for this case.

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Low K Dielectric Thin Film Development and High Frequency Characterization

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R. T. McGrath* — Professor

For microprocessor chips operating in the GHz range, low- dielectric constant materials need to be used in order to reduce the signal propagation time between transistors. To understand the effects of different processing techniques on dielectric properties, high frequency characterizations (GHz range) of interlayer dielectric material properties have been performed. In conjunction with low frequency (¡1MHz) measurements, the effects of various thin film patterning and processing techniques are being investigated. High frequency measurement techniques for determining the materials dielectric constant have been developed and validated in measurements made on SiO2 films. A new low k dielectric material with dielectric constants less than 3 has also been characterized. The thin film processing condition found to minimize damage will be identified and applied to other new low k dielectric materials.

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Tool Condition Monitoring

S. Jayasankar*
Graduate Student

This paper examines different methods to estimate tool wear. A comparison is made among the various methods of tool wear measurement. Tool wear is defined as the width of wear line under the cutting edge. The direct techniques used for measuring the width of wear land are microscope or online measuring computer based machine vision techniques, however these methods are inconvenient although accurate, because they interfere with the machining process.

The tool condition can be monitored by indirect methods like cutting force measurement, temperature, vibration, acoustic emission, power consumption measurements. It is known that all indirect methods are error prone, hence an attempt is made in this paper to predict the tool wear from two indirect methods, such as tool vibration and motor current and the results are fused to improve the reliability. For fusing the two signals a wavelet transform and cross correlation function are used. A novel idea of new rapid transform developed by authors for this kind of applications is presented.

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Nanoindentation of Alumina Matrix - Chrome Carbide Nanoparticles Composite

Liudmila Yerakhavets* Leading Investigator

Maksim Kireitseu* Principal Investigator

Ion Nemerenco* Investigator

The work revealed the possibility to improve physical, mechanical properties of alumina-based ceramic composite by CrC-based thin coatings produced by the metalorganic chemical vapor deposition. The CrC coatings heal various surface defects of the alumina that strengths and toughs the composite. It is found to be high microhardness and fracture resistance regarding initiation and propagation of Palmquist cracks during Vickers indentation. The nanoindentation hardness and abrasive wear resistance by dimple grinding test of the coatings were compared between the sample series and related to the microstructure, phase composition, and residual stress obtained by transmission electron microscopy, x-ray diffraction, and substrate curvature technique, respectively. All films exhibited a dense and columnar microstructure. Nanoindentation test showed high hardness for CrC alumina multilayer and homogeneous alumina in the range of 20-26 GPa. The absence of superlattice hardening in the polycrystalline alumina nanostructured multilayer is suggested to be due to micro cracking at pores and grain boundaries under the indenter tip. CrC layer filled the defects and pores might enhance crack propagation under overloaded indenter. For both series, fracture toughness was lower for the multilayer than the corresponding homogeneous films. The abrasive wear resistance of films between sample series showed a negative correlation with grain size. Composite exhibits higher scratch wear resistance compared to the alumina.

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Rheological Behavior and Model of Alumina-Polymer-Based Composites

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Maksim Kireitseu* — Principal Investigator
Ludmila Yerakhavets* — Investigator

Based on recent research of mechanical properties of alumina-based ceramics, polymers and their composites, we have suggested the following requirements to be used in the rheological model of the composite:

1. Since the composite includes a hard alumina layer and a steel substrate that exhibits plasticity, irreversible deformations have to be considered as plastic in nature. Deformations develop only after exceeding a critical yield strength for the particular layer of the composite.
2. If the stresses are smaller than the yield strength, deformations at constant stress are increased step-by-step to a final value.
3. Cyclic loading increases summarized plastic deformation of the composite.
4. Curve of deformation vs. time at constant load exhibits a linear dependence in one plotted region.
5. At unloading, the retardation of deformations (elastic return) has to be observed.
6. Stress at constant deformation is relaxed.

Along with the above stated items, it is important to use the following mathematical requirements: (a) the order of a required differential equation on stress and deformation should not exceed the number of possible conditions of physical limitations; (b) the system and formulated problems have to be solved concerning stress or strain rate.

The model for the studied composite material is selected by comparison of developed models and experimental results. The composite of hard alumina-aluminum can be represented with an elastic-tenacious-plastic rheological model. The polymer layer can be represented by the rheological model consisting of two elastic elements and one tenacious element. As a prototype of the model, we can consider the connection of Maxwell's model and an elastic element. The plotted relations of experimental data and calculated data have revealed very close agreement of the developed rheological model and real mechanical behavior of the composite. The above stated conditions are used in investigations of mechanical and rheological properties of the alumina-aluminum-polymer-steel composite systems. The rheological properties and perspectives to be considered in the development of such composite bearings shall be discussed.

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Synergistic Enviro-Mechanical Degradation Kinetics and Acceleration

(Symposium No. 19)

Organizers:
John J. Lesko, Virginia Polytechnic Institute and State University
Andras Szekeres, Technical University of Budapest

Strength and Durability of Graphite/Epoxy Composites Under Hygrothermal Conditions

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Graduate Student

Scott W. Case*
Assistant Professor

As composites are being increasingly used in marine environments, the necessity to understand the effects of hygrothermal exposure on the strength and durability of composite materials has become a critical issue. While much work has been done to evaluate the moisture absorption behavior of composite materials, relatively little work has been done to explore the effects of combined moisture and elevated temperature conditions on the durability of composite materials. Weitsman et al. [1,2] have shown that moisture can either enhance or reduce the fatigue life and fatigue damage of polymer composite specimens depending on test conditions. In the current study, the effect of moisture and temperature, combined and individually, on fatigue damage and durability of cross-ply graphite/epoxy composite specimens will be evaluated. Results from fatigue testing in ambient and elevated temperature water will be presented as well as corresponding dry fatigue testing results. Fatigue damage in each of the cases will be assessed and compared and the results will be used to gain an understanding of how such conditions may be incorporated in fatigue life prediction.

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Mechanical Behavior of Center-Hole Notched Nicalon/Silicon Carbide Ceramic Composites

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Assistant Professor

In this paper the mechanical behavior of center-hole notched SiC/SiC composites under quasi-static tension and stress-rupture will be discussed. The stress concentration produced by the hole affects the extent of matrix cracking and results in stress redistribution. This redistribution must be accounted for in order to produce lifetime and durability predictions. A finite element model based in ANSYS is used to model this stress redistribution and also incorporates creep and rupture mechanisms at elevated temperatures. A damage tolerance code is used in conjunction with ANSYS to predict the creep and rupture lifetime behavior of notched specimens using the behavior of unnotched coupons as inputs. The analysis is validated with stress-rupture tests at 1000 deg. C on Hi-Nicalon/Enhanced-SiC coupons provided by Honeywell Advanced Composites.

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Development of Service Life Prediction & Accelerated Aging Methodologies for Glass/Thermosetting Composites

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John Lesko† Associate Professor

Although fiber reinforced polymer composites present great advantages in strength and weight reduction in structural applications, their corrosion resistance characteristics have driven high volume use in the chemical industry. Polymeric resins (epoxies and vinyl ester resins) provide corrosion resistance to composite products used where other material systems do not possess the needed durability. While there is large volume use of these corrosion resistant systems in our industrial and national infrastructure in light structural applications, many engineers are hesitant to design with these material systems in more critical applications due to a lack of design knowledge when dealing with durability.

We seek in this program to develop a method for life prediction of glass/thermosetting composites subjected to moisture/chemical. We will focus on the durability and chemical resistance of epoxy vinyl ester resins and their composites. Degradation kinetics will be investigated on a species basis with the goal of generalizing strength loss (weeping failure and tensile/flexural capacity) under single and combined environments with various chemical corrosive species. Accelerated aging methods are sought that will allow for the estimation of residual properties given a general set of conditions without the need for customized testing regimes. Ultimately we seek to develop an engineering tool based on the load and resistance factor design (LRFD) methodology that will enable the design engineer to estimate service life based on a desired reliability. This tool will serve as a practical tool through which the fundamental science developed in this program will be organized for national and industrial use.

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Moisture Absorption and Strength Characterization of Hygrothermally Aged Pultruded Vinyl Ester E-Glass Laminates

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The purpose of this research on hygrothermal aging of vinyl ester resin and pultruded vinyl ester E-glass laminates is directed toward the prediction of strength degradation over long-term environmental aging of infrastructure composites in a finite difference diffusion/finite element stress code. Moisture absorption and strength/stiffness reduction curves as a function of water immersion temperature (RT to 80C) and time (up to 600 days) were collected for 14 layer (0/90/CSM) pultruded laminates and 2 to 4 layer (0)s, (0/90)s, and (CSM)s model composites. Moisture absorption revealed non-Fickian or a double exponential Langmuirian behavior in neat resin, clay filled resin, model and pultruded laminates. Arrhenius analysis on the peak time versus inverse temperature for the 55C through 80C revealed that equilibrium or peak moisture content would not result for 21.6 years at 25C, 8.7 years at 35C and 3.7 years for 45C immersion. With only 8 to 45% of the moisture temperature curves elapsed for the 25C to 45C data, curve fits at these lower temperatures would result in high error with the 4-parameter Langmuirian. Therefore while using Fickian diffusion analysis, the moisture-temperature curves were still clearly represented by an Arrhenius relationship for both: the diffusion coefficient, D, and the maximum moisture content, %MC. Tensile strength reduction versus time was also shown to be fit with a double exponential decay similar to the Langmuirian diffusion solution and the temperature dependence on the characteristic time terms was also characterized well by an Arrhenius relationship. Finally, a linear relationship was noted when tensile strength versus moisture content was plotted.

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Thermo-Mechanical Problems

(Symposium No. 20)

Organizers:
Panagiotis Michaleris, The Pennsylvania State University
Nicholas Zabaras, Cornell University

Computational Design of Multi-stage Deformation Processes*

Nicholas Zabaras† Shankar Ganapathysubramanian*

Professor Graduate Research Assistant

A review will be provided of recent advances towards the development of a mathematically rigorous parameter and shape continuum sensitivity method (CSM) for large deformations of hyperelastic-thermo-viscoplastic materials using an updated Lagrangian framework [1]. The continuum sensitivity analysis is performed in an infinite-dimensional continuum framework that accounts for the non-differentiable nature of the frictional and contact conditions. Coupled workpiece/die CSM analyses will be discussed appropriate for die and preform design problems.

A framework will then be presented for the sensitivity analysis and computational design of multi-stage forming processes [2]. Multi-stage design is essential in many practical applications as it provides us with a flexibility for a better control of shape and properties in the product. It will be shown that the CSM for multi-stage processes takes a similar form to the updated Lagrangian sensitivity analysis of single-stage deformation processes.

We will conclude with various examples in the design of multi-stage deformation processes.

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3-D Fracture Analysis of I-Beams with Fillet Welds

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Graduate Student Professor

Finite element analysis of transverse cracking in the vicinity of long longitudinal fillet welds in stainless steel I-Beams is presented in this paper. Transverse cracking in welded I-Beams subjected to cyclic bending is strongly influenced by the residual stresses that arise during GMAW (Gas Metal Arc Welding). Since the crack shape and growth is affected by the detailed residual stress state, accurate fracture analysis first requires a full finite element simulation of the welding process. Welding simulation yields transient temperatures and the residual stresses in the plane of the crack after cool down. Once the residual stresses due to welding are known, stress intensity factors can be computed along the transverse crack front by superposition with the bending stresses. The welding simulation uses a double ellipsoid model of a moving heat source to simulate the heating during deposition of the fillet welds. As the welds cool, high longitudinal tensile stresses cause the fillet regions to yield and the web and flanges of the beam are subjected to compressive stresses. Subsequent computation of the stress intensity factors for cracks in the plane normal to the beam cross-section is handled using enriched 3-D crack tip elements. These specialized elements, which contain the correct asymptotic crack tip displacements and strains, do not require the generation of a specialized tunnel mesh along the crack front. Thus, automatic meshing results in finite element models that provide highly accurate stress intensity factors. Relationships between the various welding parameters and the resulting stress intensity factors, for various shaped crack fronts in the beam cross-section, is examined and compared to experimental data.

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Sensitivity Analysis and Optimization of the Thermo-Elasto-Plastic Process with Applications to Welding Side Heater Design

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Pan Michaleris† Assistant Professor

Thermo-elasto-plastic material processing results in permanent transformation of the substrate. For example, processes such as welding and laser forming cause the material to have a permanent distortion and residual stress. These permanent transformations are dependent on the design variables of the process. In order to obtain desired permanent transformations of the material, mathematically and physically validated computational optimization methodologies are required.

Finite element formulations for the quasi-static thermo-elasto-plastic process in Lagrangian reference frame have been widely used. The thermal analysis is assumed to be transient while the elasto-pastic quasi-static. Thermo-elasto-plastic processes are typically assumed to be weakly coupled so that a heat transfer analysis is performed initially, and the results are imported for the mechanical analysis.

Numerical optimization methods require the sensitivity evaluation of the solutions with respect to each design variable. In the sensitivity evaluation, analytical methods give more accurate results and computationally more efficient than the finite difference method. The direct differentiation method is computationally more efficient than the adjoint method if the problem has more constraints than design variables.

In this research, a computational scheme is developed to optimize the design variables of the quasi-static weakly coupled thermo-elasto-plastic process in the three dimensional Lagrangian reference frame. Sensitivity formulations are developed from the finite element analysis equations using direct differentiation method. These formulations are used to optimize the dimensions of side heaters in the transient thermal tensioning welding process for minimum residual stress. The results of direct sensitivity analysis are validated by comparing with those of finite difference sensitivity analysis. Optimization is performed using the BFGS line search method.

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Coupled Solid State Diffusion and Mechanics in a Field Formulation

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Asst. Professor

This work represents a first step toward the development of a continuum field formulation for the coupled phenomena of diffusion and mechanics in polycrystalline solids. The basis of the formulation lies in lattice-level mechanisms, from which is built a continuum thermodynamic description of processes at micron length scales. Considering self-diffusion, the composition problem is posed in terms of a binary vacancy-atom mixture. For mechanics, isotropic linear elasticity and isothermal conditions are assumed. The coupled constitutive relations for composition and mechanics are formally derived from the underlying thermodynamics. When applied to governing partial differential equations for each subproblem, the fully coupled nature is realized. Under applied tractions or intrinsic stress, the atoms diffuse—in general from surfaces with compressive normal traction to those with relatively tensile normal traction. The flow is also mediated by electric fields via the mechanism of electromigration. In the case of metal interconnect lines in integrated circuit devices, the results of these microscopic processes are manifested in phenomena such as diffusional creep, hillock formation, grain growth, grain boundary motion, void formation and void evolution. These phenomena have a significant impact on the function, performance and failure of metal lines. A computational framework based on the Finite Element Method has been developed to solve the coupled equations. Several numerical examples are presented and comparisons with analytical results are provided where the latter are available.

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Development of Inhomogeneous Response in an Elastomeric Component Due to Thermally Induced Scission and Healing

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When an elastomeric material is deformed and exposed to a sufficiently high temperature, macromolecular network junctions undergo time dependent scission. The molecules then recoil and re-crosslink to form a new network with a new reference configuration. The material system then consists of molecular networks with different reference states. These microstructural events affect the stiffness of the material system, induce anisotropy and result in permanent set on removal of the applied force. A constitutive theory has been developed, based on experimental data and the two network theory of Tobolsky, which accounts for this temperature dependent microstructural change on the mechanical response.

This constitutive theory is used to model the response of an initially homogeneous elastomeric layer that is subjected to shear traction and heat conduction. Initially the layer is free of traction and at a uniform temperature that is low enough that there is no scission. Traction is then applied to the layer, the temperature at the upper boundary remains constant and the temperature at the lower boundary is increased to a high temperature for a period of time and then is returned to its initial value. The high temperature is in the range where there is scission and re-crosslinking. The particles thereby experience different histories of shear, temperature and scission and re-crosslinking. When layer is traction free and again at its initial temperature, it has a permanent inhomogeneous shear and acts as an inhomogeneous nonlinear elastic material. The shear stress-shear relation for this elastic response is determined and the properties of the elastic response are discussed.

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Thermal Fields Caused by Point Sources in Multiply-Connected Inhomogeneous Regions

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Professor

The response of a body to a unit point concentrated heat source is conventionally referred to, in thermal sciences, as the influence function of a point source. In mathematics, in turn, this is identified as the Green's function or matrix of a certain boundary (initial-boundary) value problem for an equation or system that simulates the heat conduction phenomenon. The role, which these functions play in both theory and applications, cannot be overestimated [1,2]. Note, however, that there is a limited number of Green's functions, whose available for engineers compact representations can be found in literature. Even in the relatively simple case of Dirichlet problem for Laplace equation in two dimensions, there are only a few regions of standard shape, for which their Green's functions are expressed in terms of elementary functions and are, therefore, appropriate for immediate computer implementations in engeneering sciences. Even the classical double Fourier series representation of the Green's function for Dirichlet problem over rectangular region cannot be considered perfectly computable because it does not allow any differentiation frequently required in practice. In the author's earlier works (see, for example, [3]), an extension was proposed of the Green's function notion so that it becomes appropriate for problems posed over piecewise homogeneous media. Accordingly, the influence function of a point source for a region occupied with a piecewise homogeneous material is referred to as the matrix of Green's type (MGT) for the governing boundary-contact value problem. Some accurately computable expressions of MGTs for steady-state problems can be found in [3]. The emphasis in this study is on steady-state heat conduction problems for 2D regions occupied with piecewise homogeneous materials. Some new MGTs are derived for simply connected regions. In addition, an algorithm is developed that is suitable for obtaining highly accurate representations of MGTs for problems formulated on multiply connected piecewise homogeneous regions. Different boundary conditions can be imposed on the contours of the considered region and the ideal thermal contact is assumed on material interfaces. It is also shown how MGTs can be used to accurately compute thermal fields generated in considered regions by heat loadings other than point sources. A number of illustrative examples are shown.

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Implementation of Eulerian Finite Element Formulation on Modeling Laser Forming

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The laser forming process is a transient heat transfer and quasi-static elasto-plastic problem. Finite element modeling of laser forming requires the use of 3D models to accurately capture the plate stiffness and curvature. However, due to the character of transient analysis, a Lagrangian model requires a uniform fine mesh along the heating line and a time- incremental approach. Therefore a 3D Lagrangian model may involve thousands of degrees freedoms and time increments for a large-scale problem, which may be computationally prohibitive.

An Eulerian finite element formulation is based on a moving configuration. For a constant moving velocity and steady output of laser, the laser forming problem can be reduced to a steady state thermal and static elasto-plastic problem. Taking this advantage, an Eulerian model does not require uniform mesh and time-increment approach. Therefore, the number of degrees of freedoms is decreased greatly and high computational efficiency is achieved.

Both Eulerian and Lagrangian approaches have been applied on modeling laser forming process. 3D Eulerian and Lagrangian finite element models of various lengths have been evaluated for simulation. It is possible to obtain a reasonable solution within relatively much shorter time by using Eulerian approach than Lagrangian approach, especially for the long parts, which are common in the real production. The Eulerian approach is nearly 2 orders of magnitude faster than Lagrangian approach. The Lagrangian analysis results indicate that the specimen length has significant effect on the angular deformation of the plate in the laser forming process.

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Ultrasonic NDE

(Symposium No. 21)

Organizers:
Joseph L. Rose, The Pennsylvania State University
Chiaki Miyasaka, The Pennsylvania State University

Singular Solution of an Integro-Differential Equation in Elastodynamics

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Visiting Researcher

Y. C. Angel†
Professor

The propagation of steady-state time-harmonic waves in an unbounded elastic solid containing cylindrical cavities that are randomly distributed in a slab region is investigated. The solid is homogeneous and isotropic on either side of the slab. A general equation for the coherent motion in the solid is derived in terms of the average exciting displacement near a fixed cavity. As in Foldy's approach, it is assumed here that the average exciting displacement near a fixed cavity is equal to the average total displacement. The equation for the coherent motion reduces to an integro-differential equation, which is solved in closed form by using a Fourier transform technique. The closed form solution greatly reduces the risks of difficult and expensive computations of the numerical solution of the integro-differential equation and allows the evaluation of the amplitudes and phases of the reflected and transmitted waves outside the slab. Inside the slab, it is shown that the second derivative of the displacement has square-root singularities near the boundary of the slab region. This work is of interest in ultrasonic evaluation and seismic exploration of geomaterials.

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Phenomenally High Transduction Piezoelectric Transducers and Introduction of Non-contact Ultrasound Analysis

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Director R&D

Though ultrasound has been in use for NDE since the early 1900s, yet its modus operandi has remained virtually stagnant. That is, test media is physically coupled and analysis is not at par with other wave-based characterization methods (Characterization of Materials, National Academy of Sciences & Engineering report, MAB-229-M, 1967.) To eliminate transducer coupling to the test media, the key requirement is extremely high efficiency transducer for ultrasound transmission in air or other gases. Our 20 years of struggle in this area has finally culminated into piezoelectric devices characterized by nearly 100% transmission of ultrasound into gases (US and International patents.) Non-Contact Ultrasound (NCU) transducers have been produced between ¡50 kHz to ¿10 MHz. Typically, the sensitivity of NCU transducers is 10 dB to 30 dB lower than conventional contact transducers. This phenomenally high transduction efficiency is sufficient to break the equally phenomenal acoustic impedance mismatch between air and solids, thus making highly desirable NCU analysis a reality. In this paper we provide the characteristics of transducers and evidence of their high transduction efficiency. Analogous to other wave-based methods, we also introduce a non-contact analyzer (US patent) for materials characterization, aimed at measuring velocity, density, time-of-flight, thickness, attenuation, defects, texture, internal and surface imaging, etc., of practically any solid, liquid, gases, or their combinations.

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A Novel Technique with Magnetostrictive Transducers for Dimensional Analysis of a Distant Specimen

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The purpose of this research was to develop a technique to measure the length change of a 15-cm. zircaloy plate in an isolated environment using ultrasonic waves. Direct contact transducers and immersion ultrasonic techniques were unsuitable for this measurement because operant conditions prohibit direct contact between a transducer and the plate. The ultrasonic waves must travel a distance of nearly 10 meters from a transducer to the zircaloy specimen. A zircaloy wire (1 mm in diameter) connected to the specimen provided a path for this signal transmission. Previous research has shown that magnetostrictive transducers, which operate at a frequency of 0.1 MHz, provide an effective means to transmit a longitudinal ultrasonic signal through wave-guides. In this experimental setup, a magnetostrictive transducer, operated in pulse-echo mode, generated longitudinal waves in a remendur (50% Fe 50% Co) rod, 1.4 mm in diameter and received the echo from the end of the zircaloy plate. The remendur wave-guide was coupled with the 10 m. zircaloy wire to transmit the signal into the specimen. This coupling was achieved by insertion of the zircaloy wire into a hole of 1 cm. depth in the end of the remendur rod. Data showed a 1.14 dB loss in signal intensity across this boundary and through the wire. At the wire-plate boundary, a coupling similar to that of the wire and remendur was achieved by inserting the wire into the plate. Attenuation in the plate and internal reflections in the remendur hindered the quality of the desired signal from the zircaloy plate. Other methods of optimizing this signal were explored. Such methods include coupling the wire and plate with a zircaloy horn and launching surface waves rather than longitudinal waves into the zircaloy specimen. With an optimized signal, this technique was quite effective for the measurement of dimensional changes in a distant specimen.

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Thermal Deformation of Alumina (Al2O3) Substrate During Soldering

Bradley Bond*

Undergraduate

Ceramic substrates play a very important role in the electronic component industry, but are very brittle and susceptible to cracking and failure. It has been shown that they may fail during the laser drilling process, but there is also potential for failure during the soldering process. Large localized thermal stresses created by the soldering iron will cause small out of plane displacements, which may lead to cracking or failure. It is difficult to measure thermal stresses in materials because high temperatures often influence the measuring devices themselves, and they create displacements of only several microns. For this experiment the electronic speckle pattern interferometry (ESPI) system was chosen because of its unobtrusive nature, high resolution, and immunity to temperature. The thermal stresses in the ceramic caused by the soldering iron will in turn cause an out of plane deformation in the substrate. These deformations can be measured using the ESPI system and used to gain information about the stresses in the ceramic. The samples being tested are ceramic Alumina substrate (Al2O3). The ceramics were clamped at both ends, and subjected to thermal loading via a soldering iron. The iron was held several millimeters from the sample for up to five minutes to simulate the soldering process. Irons of various powers were used to compare the effects of the different temperatures. During this heating process, the ESPI system, which is powered by a 15mW CW Helium-Neon laser, is running and the CCD camera is sending real time speckle images to the computer. Afterwards, successive speckle images are subtracted from one another using commercial software, resulting in displacement fringes. Information about the fringes, such as size and spacing, can then be used to calculate the out of plane displacement in the ceramic, and the thermal stresses that caused it.

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EMAT Technique for Detection of Flank Cracks in Locomotive Wheels

Subash Jayaraman*

Graduate Student

Surface and sub-surface cracks in locomotive wheels might lead to their catastrophic failure. The current methods for crack detection in railroad wheels including visual inspection, dye penetrant and magnetic particle evaluation, are archaic, time consuming and require highly skilled operators to perform and cannot detect cracks beneath the surface. All methods require at least 20 hours of work per locomotive, as the wheels must be removed and carefully cleaned. This paper exhibits the principle, application and advantages of electro-magnetic acoustic transducer (EMAT) technique in locomotive wheel crack detection. Longitudinal and Shear wave EMATs were used to detect surface, sub-surface and internals flaws, depending on the flaw characteristics.

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Elastic Properties of Organic Thick Film by Microscopy

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Graduate Student

Organic thick coatings (epoxy, polyurethane, and acrylic-urethane) have been widely applied on high modulus substrates (e.g., steel) for anticorrosion protection, and to improve their performance, reinforced components (clay, bochmite, nanopaticles, etc.) are usually added to these coatings. However the acoustic evaluation of these coatings is difficult because of their low acoustic velocity and high attenuation coefficient. In this paper, first, scanning acoustic microscope (SAM) operating frequency at about 100MHz (pulse mode) is used to image sub-surface, coating/substrate interface and to measure acoustic velocity, different phase can be observed on some coatings and infects can be found at some interfaces. Second, atomic force microscope (AFM) is applied to image surface at high resolution (compared to SAM), results agree with SAM images. Third, nano-indentation technique is utilized to measure reduced Youngs modulus and absolute hardness of coatings. Results show that epoxy has highest Youngs modulus and acrylic-urethane lowest. Reinforced components can either increase or decrease Youngs modulus and hardness depending on coating material. Finally, results from SAM, AFM and nano-indentation are compared and analyzed to optimize the evaluation.

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Analysis of Flexural Mode Tuning by Semi-analytical Finite Element Method

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Ph.D. Professor

Since thousands of miles of tubing and piping are used in all sorts of power generation, petrochemical and manufacturing plants, rapid nondestructive evaluation has become an important subject to reduce inspection time and costs. Guided waves have a great potential for the rapid ultrasonic NDE due to its prominent characteristic of long-range propagation. However, since guided waves in a pipe show very complex propagation characteristics, it should be tuned for the application to the NDE. For partial defect detection in a pulse-echo configuration, ultrasonic waves should focus on the defect to obtain large reflection. For abnormality detection in a pipe with an elbow by a through-transmission test, waves should become an axisymmetric mode after the elbow for easy analyses. In this study, a semi-analytical finite element analysis revealed the potential of such flexural mode tuning technique for the NDE. The semi-analytical finite element method can analyze very long pipes since it analytically treats guided waves as a superposition of orthogonal functions in the longitudinal direction. For straight pipes, the one-dimensional semi-analytical finite element method was used, in which a region of a pipe is divided into the cylindrical subdivisions in the thickness direction. The waveforms in the circumferential and longitudinal directions are analytically described. For a curved pipe, the two dimensional semi analytical FEM, where a cross section of a pipe is divided in the thickness and circumferential directions, was adopted. Curved regions are described by a quasi-cylindrical coordinate system where the longitudinal axis is curved along the curved region, instead of along a straight longitudinal axis. Focusing phenomena in a straight pipe were experimentally observed as predicted in a semi-analytical FEM calculation.

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Application of Nonlinear Acoustic Effect for Degradation Estimation of 2.25Cr-1Mo Steel Used at High Temperature

Ik Keun Park* Joseph L. Rose†

Professor Professor

Nonlinear acoustic effect has been considered as an effective tool for the evaluation of material degradation In this study, ultrasonic NDE for degraded structural materials used at high temperature is discussed. Especially, the feasibility of nonlinear acoustic effect to the evaluation of degradation of 2.25Cr-1Mo steel is verified experimentally. Sixteen kinds of 2.25Cr-1Mo steel specimens with different degradation levels which were prepared by the isothermal aging heat treatment at 650were evaluated by ultrasonic NDE investigating the change of attenuation coefficient, amplitude spectra, and nonlinear acoustic parameter etc. As carbide precipitation increase and spherodization near grain boundary of microstructure to aging degradation, attenuation coefficient had a tendency to increase as aging time. In addition, ultrasonic nonlinear parameter was quantitatively measured by bi-spectrum and power spectrum. Nonlinear acoustic parameter from bi-spectrum was found to be clearly sensitive to the material degradation.

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Damage Healing in an AS4/PEEK Composite Plate

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Graduate Student

Research efforts are being carried out to determine the possibility of using a CF/PEEK laminated composite in the first stage of turbine engine blades. These engine blades get damaged by low velocity impacts due to debris on runways, bird strike, tool drop etc., (impactor velocities of less than 100 m/s are defined as low velocity). A study was carried out to determine the feasibility of healing damage in an AS4/PEEK composite plate. Images of the samples were obtained using the air-coupled ultrasound technique before they were impacted to ensure that the samples were free of any gross defects. The composite plates were then impacted with a low velocity drop-weight at an incident energy of 2.26 ft-lb. Ultrasonic C-Scan system was utilized to obtain images of the impacted specimens. This was followed by the healing process, which was achieved using controlled temperature and pressure. The healed samples were imaged using C-Scan system and the results obtained by analyzing the images show a reduction in the size of the damaged area and occurrence of healing.

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Guided Wave Scattering in a Plate Overlap

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Professor

In this study, scattering of Lamb and shear horizontal waves in a plate overlap is investigated. Scattering field for Lamb and shear horizontal waves over an overlap region are numerically calculated using a Hybrid Boundary Element-Finite Element method. In the numerical study, transmission and reflection factors of the incident A0 and S0 mode Lamb waves and n0 mode shear horizontal wave across the overlap region are calculated as a function of frequency and overlap length. Scattering of higher modes produced by mode conversion phenomena within the overlap region are also included in the numerical study. Experiments are also conducted for measurements of transmission and reflection factors for incident S0 and A0 mode Lamb waves and n0 shear horizontal wave in overlap-shaped steel plates with two different overlap areas. The numerical and experimental results can be used to establish guidelines for NDE in overlapped plates and in multi-layer structures with various joints by selecting modes and tuning frequency.

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Ultrasonic Inspection Using Phased Array Systems

Paul A. Meyer*

The use of ultrasonic nondestructive inspection is well known. Critical components in power generating stations, aerospace vehicles, and chemical plants undergo regular inspections to determine suitability for continued service. Originally, inspections were conducted by an operator who manually scanned a probe over the structure and noted regions with indicated flaws. Although effective at locating flaws, the process was time consuming. Eventually, mechanisms were developed to automate the probe manipulation and test times were reduced. Still, the mechanisms had to be reset every time the geometry of the component changed. With the advent of electronically phased array ultrasound systems, the inspection process has taken another step forward. These systems can alter the location, direction, and focal characteristics of the ultrasonic beam very quickly. The scanning mechanisms are eliminated and setup changes requires by component geometry changes can be implemented almost instantly.

This presentation reviews the theory of operation of ultrasonic phased array systems and also discusses signal processing methods for enhanced flaw detection, imaging, cost-effectiveness, and operating speed.

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Improved POD Methodology for Inspection Reliability Assessment using Monte Carlo Simulation

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Joseph L. Rose†
professor

Ultrasonic inspection system is consisted of the operator, equipment and procedure. The reliability of results in ultrasonic inspection system is affected by its ability. The performance demonstration round robin test was conducted to quantify the capability of ultrasonic inspection for in-service. The small number of teams who employed procedures that met or exceeded ASME Sec. XI Code requirements detected the piping of nuclear power plant with various cracks to evaluate the capability of detection and sizing. In this paper, the statistical reliability assessment of ultrasonic nondestructive inspection data using Monte Carlo Simulation is presented. The results of the POD analysis using logistic probability model are compared to these of Monte Carlo simulation. The feasibility of the ultrasonic NDE reliability assessment is verified by the analysis of the data obtained from round robin test. In these results, Monte Carlo Simulation was found to be very useful to the reliability assessment of the small number of NDE data.

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Ultrasonic Guided Wave Inspection Potential

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Ultrasonic guided wave inspection is expanding rapidly to many different areas of manufacturing and in service inspection. The purpose of this paper is to provide a vision of ultrasonic guided wave inspection potential as we move forward into the new millennium. An increased understanding of the basic physics and wave mechanics associated with guided wave inspection has led to an increase in practical nondestructive evaluation and inspection problems. Some fundamental concepts and a number of different applications that are currently being considered will be presented in the paper along with a brief description of the sensor and software technology that will make ultrasonic guided wave inspection common place in the next century.

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Wear and Tribology
(Symposium No. 22)

Organizers:
Albert E. Segall, The Pennsylvania State University
Joseph Conway, The Pennsylvania State University

Frictional and Adhesive Properties of Diamond-like Carbon at the Nano Scale

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Diamond-like carbon (DLC) is a unique material that exhibits both low friction and high hardness. This material is being considered as a coating for a wide range of applications, including micromachines, where friction and adhesion play a critical role in performance. In the present study, we seek to understand more fully the fundamental relations that govern the tribology of DLC at the nanoscale. In particular, we wish to understand the way in which humidity tends to reduce the superior frictional properties of DLC. Coatings of DLC were deposited on silicon flats and atomic force microscope (AFM) tips using the plasma source ion deposition process. These coatings are studied using the AFM, where a nanoscale tip is placed in contact with a sample to measure adhesive and frictional forces. The experiments are performed in an environmental chamber where the relative humidity can be controlled from less than 5% to near 70%. Friction is measured as a function of load in the low load regime, to minimize or completely avoid wear. We observe a nonlinear dependence of friction upon load for silicon nitride/DLC nanocontacts. This dependence can be precisely modeled using a Derjaguin-Muller-Toporov-like contact model that takes capillary adhesion into account. The result indicates that the frictional shear strength (friction force per unit area) is independent of load, but exhibits a significant dependence on humidity, while the adhesive force remains nearly constant. We will also discuss recent results from studies of DLC/DLC nanocontacts.

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Coatings for Anti-Fretting Behavior: Tribochemistry at Fretted Interfaces

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Fretting is an interesting tribological phenomenon to understand and control. In-service fretting conditions can be difficult to simulate in the laboratory because of dynamic parameters such as amplitude, load and temperature. Of particular interest to the Air Force is fretting on Ti-6Al-4V dovetail blades in turbine engines since the surface flaws generated during fretting can initiate fatigue cracks. Fatigue cracks can result in catastrophic failure of either the blade or disk and, therefore, very conservative maintenance criteria must be imposed. Efforts are underway in our laboratory to evaluate coatings to mitigate fretting damage at these interfaces. This presentation will focus on the development of laboratory methods for evaluating fretting behavior; analytical characterization techniques to evaluate tribochemical mechanisms at fretted interfaces; and, the selection of coatings to mitigate fretting damage.

An ellipsoid on flat arrangement was developed for laboratory testing because of problems experienced with a cylindrical pin on flat configuration. The cylindrical pin resulted in non-uniform load distribution across the fretted interface that produced irregularly shaped wear scars. An ellipsoid was designed with curvature in two dimensions to eliminate alignment difficulties, creating uniform wear scars with sufficient contact area for detailed chemical and microstructural analysis. Scanning electron microscopy, energy dispersive spectroscopy and Auger electron spectroscopy were used to understand tribochemistry at fretted interfaces of several coating scenarios. Two thermal spray coatings, Al-bronze and NASA PS304, were studied at room temperature. Two hard coatings with solid lubricant topcoats, TiCN (MoS2 based topcoat) and TiC (WS2 topcoat), were also studied. Results of both thermal spray coatings show little damage to the coating; however, some surface defects were produced on the Ti64 pin. Results of the hard coating tests show that the solid lubricant does not provide any protection and that the hard coating experiences severe wear. Further work is now underway to evaluate various new solid lubricants from room temperature up to 500 C to determine their usefulness for these applications.

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Tribological Properties of Nanostructured Carbide-Derived Carbons

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Professor

In this paper, we will provide an overview of tribological behavior of carbide-derived carbon (CDC) films produced on SiC substrates by extraction of metals from carbides. The synthesis, structure and mechanical properties of carbide-derived carbons will be described. Chlorination process at 800 to 1200 C produces carbon films of various structures on SiC, TiC and other carbides [1]. Tribological tests were performed in air, dry nitrogen and high vacuum (10^{-8} torr) using pin-on-disk machines at room temperature. The test pairs consisted of a sintered silicon nitride ball (9.55 mm in diameter) and the SiC flats with and without the CDC coatings on their sliding surfaces. The effects of sliding velocity, environment (air, nitrogen, and vacuum), lubricants, and the normal force will be described. Friction coefficients of test pairs in dry nitrogen were about 0.1 (similar to that in air [2]). When SiC samples with CDC coatings were first exposed to high vacuum, and then tested in dry nitrogen, the friction coefficients became very low, i.e., 0.04 at steady states. Sliding contact tests as a function of humidity revealed the existence of a close correlation between the friction coefficient of the CDC films and relative humidity. In general, the friction coefficients decrease with decreasing humidity. Such behavior is in contrast to that of the crystalline graphite or glassy carbon, which exhibit a low friction at high humidity, but a higher friction and fracture at low humidity or in vacuum. Using Raman spectroscopy and electron microscopy, we explore microstructure and chemistry of these films and correlate these findings with friction and wear mechanisms in humid, dry, and vacuum environments.

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Failure Mechanism of Ceramic Coatings in Load Limited Scratch Tests

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Scratch tests with a spherical indenter and Rockwell indentation tests were used to study failure modes and assess adhesion to the substrate of ten different widely used PVD ceramic coatings. The coatings investigated were near frictionless carbon (NFC) coatings (NFC2, NFC6, and NFC7), nitrides of titanium (TiN-UES, TiN-DTC, TiCN, and TiAlN) and nitrides of chromium (CrN1, CrN2, and CrN3). Before subjecting these coatings to scratch tests, the Calo Test was used to determine their thickness. Three different diamond stylus radii (125, 300, and 533 microns) were used to conduct single pass scratch tests. Each test was repeated at least five times on all ten coatings. Multiple pass fatigue experiments were also carried out using the largest radii stylus. The responses measured included friction force, normal force, friction coefficient, scratch length, and acoustic energy released. An industry standard adhesion comparison test #2997 that used a rating of one corresponding to best adhesion and six corresponding to worst adhesion was used to compare the adhesion of all ten coatings. Comparison tests showed variations in adhesion from 2-4 in NFC coatings, from 1-3 in titanium nitride coatings, and a rating of 2 was observed in all chromium nitride coatings. Optical and scanning electron microscopy was used to study the microstructures of the coatings, their surface and subsurface damage patterns due to scratching, and the morphology of the ploughed debris. It was found that the damage mechanism was predominantly dependent on the microstructure of the coatings. Microfracture was found to be the predominant mechanism of material removal due to scratching and indentation in chromium nitride and titanium nitride coatings, which are crystalline in structure. In most cases, the microfracture followed the grain boundary and occasional cleavage of grain. Because these crystalline coatings have a columnar microstructure with intercolumnar region being the weakest, failure in these coatings is associated with locations of lower fracture toughness. Macrofracture was the predominant mechanism of material removal in near-frictionless carbon coatings. Fracture in the amorphous carbon coatings showed a straight trajectory and has the characteristic brittle cleavage appearance. Such fracture mode is typical for amorphous solids. The crack trajectories followed a path similar to that of maximum tensile stress cracks in elastic contact. In the present scratch test, which is a sliding spherical elastic contact, the tensile stresses are imposed at the trailing edges of the contact. Thus the fracture and crack pattern observed in amorphous carbon coatings coincided perfectly with the elastic stress field.

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Temperature-Dependent Degradation Mechanisms in Cu-Ni-In Anti-Fretting Coatings and the Complicated Search for Alternatives

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Carl Hager† — Research Scientist

While titanium alloys are often ideal for aerospace applications, they are also susceptible to fretting damage and the catastrophic failures that can follow. This is especially true for the dovetail joint between the turbine blades and disk where the temperatures and complex mixture of stresses and relative motion create conditions that are conducive to both fretting and fatigue. Because of this susceptibility, lubricious coatings such as Cu-Ni-In are often used to help delay titanium-on-titanium contact and eventual fretting. Unfortunately, micro-adhesion mechanisms appear to facilitate the direct transfer of titanium to the softer lubricious coating at the lower operating temperatures (177C) typical for the first stage fan. At the higher operational temperatures (454C) of the third stage compressor, a distinct segregation of the copper leaves the coating significantly weakened. In either case, the ability to avoid titanium-on-titanium contact is lost and fretting damage and fatigue ensues. To help simulate these complicated damage mechanism, an accelerated tribotesting procedure was developed that employs a unique combination of gross-slip reciprocating displacements ranging from 25-125mm. The test methodology was then used to assess a variety of hard and lubricious coatings at the two operational temperatures for up to 3x106 fretting cycles. As part of the study, traditional Plasma, as well as High-Velocity-Particle-Consolidation (HVPC) coating techniques were also investigated. Results indicate that the mixed range of gross-slip displacements can adequately match the observed titanium transfer, but not the copper segregation experienced by the compressor. The study also found that the fretting resistance of the HVPC coatings is virtually equivalent to that of Plasma, and that nickel and cobalt coatings applied by either method show promise. Finally, the research also indicates that the use of boron nitride as a lubricant helped reduce damage to the coatings.

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Handheld Slipmeter to Measure Slip Resistance between Shoe and Flooring Materials

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Insufficient slip resistance between shoes and flooring often causes pedestrian slips and falls. Falls are the leading cause of accidental death for the elderly; are second only to automobile accidents as the leading cause of all accidental deaths; and are responsible for 13% of accidental deaths and 17% of disabling injuries in the workplace. Unfortunately, repeatable measurement of slip resistance has historically been a problem in that the four current types of slipmeters can produce significantly different readings between different devices and between different operators for the same shoe and flooring materials. In particular, wet contaminants between shoe material friction coupons and flooring samples can cause spuriously high readings for horizontal pull and older articulated strut slipmeters that inherently have longer contact times between the friction coupon and flooring. To this end, a new handheld electronic slipmeter was developed for accurate and repeatable measurement of coefficient of friction (COF) between shoe and flooring materials under dry and wet conditions. Design issues and calibration procedures for this microprocessor-based slipmeter are presented. The design incorporates a leading fixed-fixed cantilever beam and a trailing fixed-fixed cantilever beam between the friction coupon and a pivot block. Both the leading and trailing beams are instrumented with strain gages. The pivot block allows free rotation of the friction coupon relative to a handle that contains signal conditioning and display electronics. Vertical and horizontal forces from the handle onto the friction coupon caused by manually pushing the slipmeter down and forward on a flooring sample are measured by a microprocessor to determine COF. Validation data from a prototype handheld slipmeter and from manual horizontal pull testing using a Neolite shoe friction coupon on four ceramic floor tile samples were compared to assess efficacy. Each tile was tested three times in each of four cardinal directions for both dry and wet (distilled water) conditions. For all four tiles, dry kinetic COF measurements from the prototype statistically matched horizontal pull measurements at 0.01 significance. As expected, all wet kinetic COF measurements were significantly lower for the prototype compared to horizontal pull tests. For all four tiles, dry static COF measurements were always higher for the prototype versus horizontal pull tests while wet static COF measurements had statistically mixed results across the four tile samples. Repeatability of dry COF measurements with the prototype handheld slipmeter was very comparable to repeatability for horizontal pull slipmeters specified in ASTM standard F609-96.

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Measurement of Interfacial Wear using Focused Ion Beam Milling

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The primary goal of nanoscale interface tribologists is to develop interfaces that support contact while limiting interfacial wear to only several nm. Accurately measuring wear at the nm scale is one of the biggest challenges to this development. We describe a method of creating surface fiducial marks on the surface of an air bearing slider in the area in which most wear occurs and using these to quantify wear. Marks are made using focused ion beam (FIB) milling, have very repeatable dimensions, and can be made as shallow as several nm. Milled sliders underwent slider-on-disc wear testing, in which sliders were contacting lubricated and carbon-overcoated metal surfaces. Disc drive tribology testers were used to perform testing and conditions reproduced conditions inside a disc drive. Test linear velocity was 750 inches per second and the load force was 2.5 grams. During testing, slider dynamics were measured using laser Doppler vibrometry, which we use to measure the vibration spectrum of head motion and to give insight into how the head is responding to contact. Test duration was varied to identify trends in the locations of wear. Atomic Force Microscopy was used to measure the change in height of worn surfaces relative to the unworn FIB marks, which gives a direct measure of wear. We report correlations between the magnitude of slider vibration and overall amount of wear and between specific head motions and wear patterns on slider surfaces. Through this approach, we relate how variations in slider pitch angle (both static and dynamic pitch angles) relate to wear patterns at the slider trailing edge.

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Micromechanical Modeling of Contact/Friction in Ceramic Materials Under Pressure-Shear Loading

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A grain level microstructure model is presented to analyze micromechanical behavior of friction and wear in ceramics. A basic understanding of frictional behavior at interfaces is gained by performing dynamic pressure-shear plate impact experiments on thin ceramic specimens sandwiched between hard tool steel plates. The developed computational model is utilized to investigate the features observed in pressure-shear interferometric signals. This combined experimental/computational approach is used to model inelasticity in microstructured materials and examine the role of interfacial friction in the interpretation of pressure-shear experiments.

The investigation consists of analyzing the relative effects of ceramic microcracking, temperature rises, plastic flow in the steel plates, and frictional deformation and sliding at the interfaces between ceramic and steel anvils. A surface-defined multibody contact algorithm designed to handle large relative displacements between bodies is employed. The grain model incorporates interface cohesive laws to capture microcrack initiation and propagation in the ceramic. Representative volume element calculations of random microstructures are performed to obtain insight into the effects of grain size and morphology as well as distribution of chemical impurities and glassy phase. The investigation is extended to the study of plastic flow in the steel plates by accounting for visco-plasticity, thermal softening, and strain hardening. The model also employs a surface roughness typical of manufacturing processes to capture the time dependent frictional behavior.

Pressure-shear impact velocity histories are used to identify inelasticity as well as to determine dominant failure modes as governed by bulk and surface properties. It is identified that frictional effects play a dominant role in the observed velocity histories and that the design of experiments to interrogate the bulk properties of hard materials, under combined loading and finite deformations, remains a challenging task. The proposed model is found to be capable of predicting the role of local inelasticity in the frictional behavior of interfaces as functions of surface characteristics. Applications such as ceramic machining and turbines can be studied within this model framework.

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Simulating the Contact and Interaction of Engineering Surfaces

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Surface interaction actually results from the contact and rubbing of asperities. Understanding the performance of surfaces in a Tribological process requires the information of the thermomechanical status of asperity interaction. With the assistance of powerful analytical tools, such as Greens functions and the Fourier transforms, we have developed effective numerical algorithms and a set of thermomechanical asperity contact models that can be used to simulate the performance of rough surfaces in contact and relative motion. Reported here are the algorithms of our discrete convolution and FFT (DC-FFT) method, formulations of the asperity contact models, and simulations of the thermomechanical contact of rough surfaces under translation/reciprocating motions.

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Wear Evaluation of HIP Compacted, Nitrogen Enhanced, Atomized Stainless Steels

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High nitrogen stainless steels are a class of materials that demonstrate an attractive combination of strength, ductility, and corrosion resistance properties. Rapid solidification that occures during atomization introduces additional benefits such as increased nitrogen concentrations, enhanced microstructural refinement, and chemical homogeneity. HIP consolidation allowed the powders to form solid compacts without formation of nitride precipitates. Mechanical properties show these materials to have HV(1000)hardness in excess of 300, yield strength greater than 600MPa, UTS greater than 1000MPa, longation greater than 50%, and impact energies greater than 100J. These materials have also been shown to have excellent corrosion properties. The above results suggest that these materials may be excellent canidates for medical implants. To evaluate the wear properties of these materials, (i) diamond single scratch, (ii)pin-on-abrasive disk, and (iii)metal-metal pin-on-drum in Ringers solution wear tests were conducted. In addition to evaluating the as-consolidated material wear properties, two surface treatment were applied and wear tested: shot-peened surfaces and surfaces coated with TiN. To further evaluate these high nitrogen steels, wear tests were 316 stainless, 440C and Co-Cr-Mn steels.

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The Influence of Manufacturing Processes on the Reciprocating Wear Behavior of Hypereutectic B390 Alloys

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An understanding of the abrasive and sliding wear behaviors between alloys such as aluminum (piston) and cast iron (engine block) are of obvious importance to the automotive industry. Because of the sometimes contradictory requirements between reduced weight and wear resistance, this research involves the development of light-weight and wear resistant alloys including new manufacturing methods and relevant wear testing. As a result, hypereutectic B390 alloys manufactured via casting, spray forming, spray forming with extrusion, and semi solid forming methods were evaluated. During the wear evaluation, a reciprocating cylinder on plate configuration under constant contact pressure was used to evaluate the B390 alloys. Initially, the testing protocol called for each pin specimen to be weighed and the volume loss calculated after a prescribed number of reciprocating cycles. However, it was observed that many of the pins were gaining weight during the process even though they showed visible signs of wear. A closer inspection revealed that cast-iron debris was adhering to the B390 cylinders during the tests and obscuring the actual wear rates. To compensate, the aluminum volume was directly determined from the changing geometry of the worn flat on the cylinder after each test sequence. Results of the tests indicated that the spray formed, spray formed then extruded, and semi solid formed all experienced approximately 20% decrease in their wear rates relative to the cast B390. However, despite their microstructural differences, there were not any significant disparities in the observed wear rates between the spray formed and semi solid formed hypereutectic alloys, even after extrusion. Hence, it does not appear that the various manufacturing processes had a profound effect on the reciprocating wear resistance of B390.

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Lubrication Issues in Aircraft Hydraulic Pumps

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High-pressure (3000-4000 psi) hydraulic systems are generally used on an aircraft to power the control surfaces, landing gears, brakes and other auxiliaries. The engine driven hydraulic pumps provide the necessary flow at these high pressures. Thus, the hydraulic pumps are the most critical component in an aircraft hydraulic system. Pressure compensated, variable flow, axial piston type design is commonly used for these pumps. The internal leakage, also known as case-drain-flow, is an integral feature of these pumps. To maintain high efficiency (low case drain flow) and durability, the pump parts have to possess tight clearances and excellent tribological characteristics. Various rolling and sliding interfaces in the pump experience a variety of lubrication regimes, namely boundary, fluid-film, and mixed lubrication. While fluid-film regime is the desired mode, boundary lubrication and mixed lubrication are encountered by most interfaces at lower speeds. The exposure of the pump parts to the different lubrication regimes makes these pumps excellent tribological specimens. The hydraulic fluid used in the system provides lubrication for various interfaces in the pump. Factors influencing the tribological performance of the pump/fluid pairs were studied, using endurance pump tests.

Endurance pump tests were conducted with fire-resistant hydraulic fluids and several candidate nonflammable hydraulic fluids using pressure-compensated axial flow piston pumps. A well instrumented, small volume, closed-loop hydraulic test stand was used. Various pressures, temperatures, flow rates, and motor torque were monitored throughout the tests. The tests were conducted at the maximum design temperature of the aircraft hydraulic system. The main flow rate was cycled between full-flow and quarter-flow every minute to increase the severity of the tests. Periodic fluid samples from the test stand were analyzed to monitor the fluid properties and dissolved wear metals. The fluids containing viscosity-index-improvers underwent large viscosity losses. No viscosity loss was observed for the fluids that did not contain the viscosity-index-improvers. Lower viscosity fluids performed as well as the higher viscosity fluids in these pump tests.

Whenever the test pump was nearing failure, certain characteristic high-frequency variations in the outlet pressure and the case drain flow, were observed. These signal fluctuations are thought to be due to the wobbly motion of the rotating pump-parts, caused by the excessive wear/spalling of the main bearing. The failures were generally captured by a sudden increase in the case-drain temperature. The thrust ball bearing of the pump and the piston-shoes experienced the most wear in these tests. The material and the heat treatment of the thrust bearing had a big impact on pump life. Use of an M-50 bearing in place of the AISI-52100 bearing doubled the pump life.

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Effects of Surface Modification on Thrust Washer Lubrication

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Surface geometry modifications such as grooves and dimples are examined as a method for designing a self-preserving thrust washer. An experimental test rig is presented that enables accurate measurements of the film thickness generated by the modified thrust washers. The measurements indicate that grooves and dimples can produce significant load support with grooves generally less sensitive to changes in speed than dimples. The larger and deeper dimples considered generate a relatively greater film thickness than shallower dimples. The density of surface features plays a negligible role in the overall thrust washer performance.

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Advanced WC-Co Composites for Cutting Tool Applications

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The study focuses on functionally graded WC-Co cutting tool inserts with residual thermo-elastic stress states tailored to counteract forces imposed by machining. Finite element analysis was employed to model both the residual stresses present in a graded tool after fabrication, and the thermal and mechanical forces encountered during machining. Processing methods were developed to fabricate laminated tools with a thin, hardened case layer under residual compressive stress. The study compares the machining performance of hot pressed and pressureless sintered inserts, as well as commercially available tools. Sintering schedules and grain growth inhibitors were tailored to achieve sintered grain sizes below 500 nm. Machining performance was evaluated through high speed lathing of 6-4 titanium. Wear rates, cutting forces, and power consumption data are compared. Functionally graded cutting tools are shown to require less power than commercial tools in cutting titanium. The microstructural features that dictate machining behavior will be described and related to processing methods. Microstructural defects, such as free carbon, have been eliminated resulting in improved cutting performance. Hardness, toughness, and elastic properties will be reported. Supported by the Center for Innovative Sintered Products at Penn State University.

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Experimental Investigation of the Effects of Feed and Speed on Exit Burr Formation in Drilling

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The formation of burrs in the drilling process has great influence on hole quality. Burrs formed at the exit of holes might cause difficulties in assembly, damage other components, and in some cases they might affect the functionality of the component or even cause injuries during part handling. Additional subsequent operations such as deburring will add to the overall cost of production. This article discusses the results of an experimental investigation to study the effect of cutting conditions (speed and feed) on the exit burr formation. A conventional uncoated High Speed Steel (HSS) twist drill (0.5 inch in diameter) was used to drill holes in low carbon steed plates. To minimize the influence of other parameters, all drilling operations were carried out with no coolant and using only sharp tools. Several combinations of the cutting speed and feed rate were used to construct a burr formation and classification chart. The exit burrs where classified based on (1) burr thickness, (2) peak burr height, (3) Burr volume, and (4) burr circumferential size around the hole (or burr uniformity), and (5) burr strength (or ease of removal). Although some of these ratings are interrelated they still give different interpretation of burr formation mechanism as it pertains to process conditions. The five measures were averaged to give a final rating for estimating a scale of best to worst classes of exit burrs. This scale was sufficient to capture the relationship between burr characteristics and the operating conditions. The chart was presented as a (feed vs. speed) matrix of collected digital images of the exit burrs. It was found that the feed rate had the most significant influence on exit burr formation. At very low feed rates the formation was minimized for almost all values of cutting speed. The worst burrs were formed at high feed rates. The relationship between the cutting speed and the burr geometry was not linear. However, burrs formed at higher speeds were more brittle and easier to break. The classification chart showed also the different geometry of burrs formed at different combinations of drilling parameters.

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X-ray Computed Tomography in Materials Science & Engineering

(Symposium No. 23)

Organizers:
Nevin L. Rupert, US Army Research Laboratory
Joseph M. Wells, US Army Research Laboratory

Image Processing and Visualization of X-ray Computed Tomography Data

William H. Green* Nevin L. Rupert† Joseph M. Wells‡

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X-ray computed tomography (XCT) is a powerful nondestructive evaluation method that is broadly applicable to any material or test object through which a beam of penetrating radiation may be passed and detected, including metals, plastics, ceramics, metallic/nonmetallic composite material, and assemblies. The principal advantage of XCT is that it provides densitometric (i.e., radiological density and geometry) images of thin cross sections through an object. Because of the absence of structural superimposition, images are much easier to interpret than conventional radiological images. The user can quickly learn to read XCT data because images correspond more closely to the way the human mind visualizes three-dimensional (3-D) structures than projection radiology (e.g., film radiography, real-time radiography, and digital radiography). Further, because XCT images are digital, the images may be enhanced, analyzed, compressed, archived, input as data to performance calculations, compared with digital data from other NDE modalities, or transmitted to other locations for remote viewing, or a combination thereof. The field of image processing (IP) of not only XCT data, but also digital data in general, is large and varied. This presentation will discuss a number of aspects of IP of XCT data, including some examples from applications studied at the U.S. Army Research Laboratory, Aberdeen Proving Ground. Single slice two-dimensional (2-D) images can be processed using averaging, median, smoothing, edge enhancement, and a variety of other filters.

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Comparison of Optical Coherence Tomography, X-Ray Computed Tomography and Confocal Microscopy Results from an Impact Damaged Epoxy/E-glass Composite

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Optical coherence tomography (OCT) is an emerging technique for imaging of synthetic materials. OCT is attractive because it combines high sensitivity (greater than 90 dB), high resolution (5-20 micron), and low cost, approximately $75 k. The value of any new technology is evaluated by how well it compares with existing methods. In this work, impact damage of an epoxy/E-glass composite is imaged using OCT, and the results were compared with micro-focus x-ray computed tomography. This technique is a good benchmark to compare with OCT because both techniques have the ability to locate features precisely and have comparable resolutions. OCT is considered to be a confocal technique so it was also compared to laser scanning confocal microscopy (LSCM). Contrast mechanisms, sensitivity, resolution, depth of penetration, and artifacts among the techniques are compared and contrasted. Also, impact damage features revealed using OCT are briefly discussed.

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The Detection of Porosity and Defects in Composite and Metal Samples with High Resolution Volumetric Computed Tomography

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A bench-top volumetric computed tomography (VCT) system has been assembled, which employs amorphous flat panel detector technology. Developed and evaluated initially for medical applications, the system is now being utilized for preliminary assessment of potential industrial applications. The configuration of the system includes a 15 cm field-of-view, based on a 20cm x 20cm 200 micron pitch flat panel detector and using a 120 kVp x-ray source with 0.6mm beam spot size. The detector includes a 420 micron thick CsI scintillation layer which provides detection efficiency of approximately 50 per cent for a 120 kVp beam. An alignment phantom with known metrology is imaged to provide geometric corrections to the reconstruction program. Magnifications in the range of 1.5-2.0 provide isotropic spatial resolution between 133 microns and 160 microns at the isocenter. Small area ($\tilde{1}$mm) constrast sensitivity of better than 1% has been demonstrated. Typical data acquisition times of 30 seconds for 1000 views provide projection data reconstructed with the FDK algorithm, including motion and alignment corrections also developed by GE. Initial low energy (120kVp) applications work has focused on the detection of porosity and wrinkles in filament wound composite samples and imaging of the fracture pattern in titanium projectile impact samples.

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Pre- and Post Nondestructive Evaluation of Ballistically Impacted Composite Helmut Using X-ray Computed Tomographic and Thermographic Analyses

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The coupling of x-ray computed tomography (XCT) established baselines with thermographic evaluation could result in a system of inspection for defective personnel protection components at the depot level by technicians with moderate training. XCT inspection was used to determine and define damage baselines within components. These baseline components were scanned using thermography to establish corresponding thermal images. The baseline components were ballistically tested to determine performance as effected by damage level. A limited catalog of thermal patterns was compiled relating the thermal pattern to components suitability for use. At the depot level thermography units could scan personnel protection components and the resulting thermal images compared with cataloged thermal images to insure components viability. This will result in lower life cycle cost and higher effectiveness of personnel protection components. This paper addresses a cursory study into the feasibility of such an approach.

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Using Topological Rule Based Algorithms to Analyze X-Ray CT Data of Composite Microstructure

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Associate Professor Professor Professor

The 3-dimensional yarn architecture in a 2-dimensional woven fabric reinforced composite is nonuniform. Structural features such as nesting and offset appear that are not obvious from consideration only of the yarn architecture in the single layer textile fabric. These conclusions were drawn from a complete set of 3-dimensional image data for a representative volume of the composite using X-ray micro-computed tomography. X-ray scans were conducted with the AEA Technologies Tomohawk CT-system implemented on a Phillips HOMX 161 microfocus X-ray system (5-160 kV, 0-3.2 mA), using a spot size of approximately 25 microns. Each pixel in the data slices is 26 microns on a side, and each slice is separated by approximately 20 microns. Extensive image analysis was necessary to reveal the yarn architecture due to relatively low signal-to-noise ratio and contrast levels relative to optical microscopy of polished cross sections. The first step in the image analysis used a relatively new denoising method based on level-sets, with a primary benefit of removing speckle noise without reducing edge definition. Due to the volume of data, automation was required to speed the feature recognition process. Automation was achieved using two concepts, propagation and iteration, which allow us to propagate identified features throughout the data set and to iteratively refine the identified features. Both the iteration and propagation operations were guided by knowledge of the fabric topology, which provided constraints limiting the number of possible ways to connect yarn segments into complete 3D yarns constituting the basic structural elements of the material. The resulting structure is being used in several investigations to predict hydraulic permeability and mechanical behavior. For example, lattice Boltzman simulations of the fluid flow in nested structures indicates a large range of possible permeability magnitude and anisotropy values. This is in qualitative accordance with large numbers of measurements conducted to develop a statistical description of the permeability for the same material used in the X-Ray study.

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Visualization of Interface Defeat Based Impact Damage in TiC Armor Ceramic

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X-Ray Computed Tomography, XCT, was utilized to nondestructively interrogate the impact damage occurring internally in a 72-mm diameter by 25-mm thick TiC armor ceramic sample. The fully constrained sample sustained the impact of a tungsten alloy sub-scale projectile with no penetration into the target sample. The tungsten alloy penetrator was completely defeated at the front surface of the TiC disk resulting in a condition known as "interface defeat" or "complete dwell". A considerable amount of meso-scale cracking of minimum dimension greater than 200 microns or 0.2-mm was detected in-situ with contiguous full cross-section XCT scans of 0.5-mm thickness. Visualization of this impact damage is shown in 2-D via XCT slices and in arbitrary multi-planar slices. Improved visualization of this damage is shown in 3-D via solid object and point cloud computer reconstructed images. Traditional types of impact cracks including conical, laminar and radial were observed but in a very asymmetric distribution. A premise is conceptualized to relate the role of the meso-scale cracking to the Sustainment and termination of the dwell condition.

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Advanced X-ray Computed Tomography at the Army Research Laboratory: Capabilities and Applications

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X-ray methods are one of the five or six conventionally considered main nondestructive evaluation or nondestructive testing areas, which also include liquid penetrant, magnetic particle (electromagnetic), eddy current (electromagnetic), ultrasonic, and acoustic emission testing. X-ray computed tomography (XCT) is a very useful x-ray method that provides information that conventional x-ray radiography, including film, real-time (fluoroscopy), and digital, cannot.

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Observations of Anomalous Internal Ballistic Damage in Monolithic Ti-6Al-4V Alloy

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The insitu damage assessment of 25-mm thick monolithic Ti-6Al-4V alloy plate material following V50 ballistic testing with both 12.7-mm hard steel and 12.7 -mm tungsten alloy projectiles was conducted via x-ray computed tomography, XCT. Selected partial penetration and through perforation samples were examined nondestructively with the 420 keV BIR CT-system at the Army Research Laboratory in APG, MD. Digital radiographs revealed the through thickness profile of the ballistic cavity and deformation and fracture of the penetrator. XCT scans were conducted perpendicular to the projectile flight direction from the entrance (impact) face to the exit face sequentially in contiguous incremental slices of 0.5-mm thickness. Several observations are made with respect to the apparent morphology of the ballistic damage in the target titanium alloy and are presented in this report. First, the diameter, smoothness and straightness of the ballistic cavity are observed to vary irregularly along the penetration depth, particularly with the more deformable W-alloy penetrator. Secondly, the presence of intermittent "orbital" cracking segments and voids is observed starting at about 60% of the sample thickness. These defects are at a significant distance (approx. 1 to 2 cavity radii) away from the surface of the ballistic cavity. Physical connectivity between this cracking damage and the ballistic cavity except near the exit face was not observed within the feature resolution limits of the XCT (greater than 200 micron), but was verified by physical sectioning and polishing. Thirdly, in the 12.7-mm steel penetrator samples, the orbital cracking segments vary in length and rotate in a clockwise spiral fashion along the penetration depth until within 2-3mm of the exit surface. No satisfactory explanation for these spiral cracking observations is presently available and neither have prior reports of the same been found in the literature. Finally, laminar density striations are observed in reconstructed images of the protruding petals on the exit surface of the APM2 samples. These striations may be related to dilatational or shear banding deformation zones created as dishing or bulging of the rear face occurred. At present, these XCT observations of ballistic damage morphology appear somewhat anomalous to those described by current models.

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Damage Assessment in TiB2 Ceramic Armor Targets: Part I X-ray Computer Tomography and Scanning Electron Microscope Analyses

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Mechnaical Engineer	Materials Engineer	Physicist	Materials Engineer

The extensive characterization of ballistic damage in ceramics resulting from impact by long-rod penetrators to aid in the design and development of improved impact-resistant materials and armor systems is presented. However, this level of damage evaluation is currently not normally done for ceramic targets. This paper discusses the damage characterization in three ceramic disks in different prestress states subjected to single and dual impacts. Evaluation of the damage includes microstructural analysis using a scanning electron microscope (SEM) with a Robinson Backscatter Detector for surface structure and an x-ray computed tomography (CT) nondestructive technique to completely scan the interior of each disk. The SEM data of the disks are compared and contrasted. The x-ray CT technique, which heretofore has not generally been used by the ballistic research community, has successfully mapped the location of impact damage and residual penetrator material within the entire volume of each disk. The mesoscale (102 mm103 mm) data of the disks obtained using the CT technique are extensively compared and contrasted. The potential for better understanding of the penetrator-ceramic interaction in ongoing and future work from extensive knowledge of the ballistic impact damage obtained by x-ray CT is exciting to the authors.

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Damage Assessment in TiB2 Ceramic Armor Targets: Part II - Radial Cracking

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The interaction between long rods and ceramics is only partially understood. However, this understanding is essential in the design of improved performance of impact-resistant materials and armor system design applications. The current work takes a preliminary look into the current understanding surrounding the formation of radial cracking in ceramics during ballistic penetration. Tests were conducted using a 32-g tungsten alloy laboratory penetrator with a length/diameter (L/D) = 20 at a nominal impact velocity of 1600 m/s. Testing evaluated both prestressed and unstressed titanium diboride ceramic tiles. The ongoing analysis of the ceramic targets includes x-ray computed tomography (CT) scans and analytical modeling of the stress state.

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General Topics
(Symposium No. 24)

Organizer:
Charles E. Bakis, The Pennsylvania State University

Non-Linear Electromechanically Coupled Modeling of Thin Piezoelastic Composite Plates

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Research Scholar

In the present paper, thin piezoelastic composite plates are studied. The modeling is characterized by the consideration of mechanical and electrical field equations. These equations are coupled to each other by means of the direct piezoelectric effect and the converse piezoelectric effect. Owing to the thinness of the plate the mechanical assumptions are based on classical lamination theory and the electrical field equations reduce to the one-dimensional charge equation of electrostatics. In order to account for the influence of moderately large deformations, we consider non-linear strains in the sense of von-Karman and Tsien.

The direct piezoelectric effect that characterizes the conversion of mechanical energy into electrical energy naturally results in the necessity of different modeling strategies for different electric boundary conditions. We analyze electroded layers with either the electric potential or the total charge being prescribed, as well as non-electroded layers. We end up with a plate model that takes into account the electromechanical coupling by means of effective stiffness parameters. In case of electroded layers with the total charge prescribed constitutive relations are found to be non-local. This brings in a new aspect into thin plate theory.

As a special case simply supported plates of arbitrary polygonal planform with the boundary being prevented from in-plane motion are studied. We furthermore restrict ourselves to plates with a symmetric lamination scheme, for which the layers are made of transversally isotropic materials. By applying the generalized Berger-approximation we end up with a suitable formulation for the analysis of the non-linear electromechanically coupled behavior of thin piezoelastic composite plates.

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Optimal Spray Patterns For Liquid Application to Structured Packing

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Professor

Various wet processing systems function by dispersing liquid streams over the top of a packed bed, so that the liquid flows down over the extended surface of the bed media to achieve a particular desired effect. Examples include evaporative cooling towers, certain reactors for chemical processing and land spreading of wastewater for treatment. A common means to disperse the incoming flow stream is a manifold of spraying nozzles, located above the surface of the bed to be wetted. Typically, such nozzles produce a circularly symmetric pattern of liquid deposition, but are arrayed on a square, rectangular or triangular grid. Because of this inherent geometric incompatibility, a symmetric but non-uniform application of liquid occurs at the top of the bed, even if the patterns from adjacent nozzles are overlapped for better coverage. This paper is concerned with methods for establishing the best possible pattern of spray flow onto packing media from individual nozzles placed in a particular array configuration. Previous investigations have developed some insights as to the characteristics of nozzles that will provide high uniformity when applying liquids to plane areas, but the more general problem of finding optimal nozzle patterns for use in conjunction with a packed bed to achieve maximum system performance has received little attention. Structured packing media (consisting of many layers of regular cells that average flows from adjacent cells above) were of special interest in the present effort. The determination of optimal nozzle spray characteristics was posed as an inverse problem and solved numerically. The spray deposition for an individual nozzle was described as a point function at a set of radial locations, subject to appropriate constraints. For a particular manifold array and structured packing configuration, the total application to the top packing layer was computed by summing the deposition of the individual nozzles. Local changes to this initial pattern were followed through the packing structure, using a detailed computational model specific to the process under consideration. The final result of liquid interactions taking place in the volume of the packing was formulated as an objective function to be minimized by variation of the nozzle parameters. Redistribution of flow in the packing and the related problem of mixing of fluid streams with chemical reaction were investigated using this approach. One important result of this investigation was the observation that nozzles developing good process efficiency do not necessarily apply liquid with high uniformity over the top layer of the packing. Thus, simply measuring the uniformity of deposition patterns on plane surfaces may not be a suitable diagnostic for system performance that is ultimately dependent on subsequent interactions in the packing. Implications for situations including liquid loss at boundaries and heat/mass transfer have also been considered.

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Thoughts on the use of Science Fiction in Engineering Instruction to Teach Basic Concepts and to Create Positive Images of the Profession

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Engineering educators must often provide new students with critical nudges to help them get it, especially in early core courses such as statics and dynamics. Furthermore, many good students loose interest in engineering because of the disconnect that occurs during the heavy emphasis on math, physics and chemistry of the freshman and sophomore years. To make matters worse, a recent Harris poll has revealed that a majority of Americans believe that the technological advances enjoyed today are primarily the result of scientists, and not engineers. While these issues do not necessarily spell the end of engineering as we know it, they do present a number of interrelated challenges for engineering educators. One intriguing remedy to many of these challenges involves the use of science fiction as seen in the movies and literature in the engineering classroom. Long used for enhancing science and physics education, science fiction has not been effectively integrated with engineering education. Unfortunately, this represents a loss of a valuable tool for enhancing the educational experience, as well as attracting new students to the profession. With these basic ideas in mind, a new freshman-level class has been developed that uses science fiction as conveyed in films and literature to illustrate and teach basic engineering concepts. Central to the course delivery is poking fun at the disobedience of the laws of physics and engineering and teaching the correct behaviors. In this fashion, students can develop lasting mental pictures of the way things function that can help with the many classes ahead. It is hoped that this approach will be especially helpful with difficult courses such as dynamics where the students often complain that they cannot visualize the motion. The novel course also discusses the implications of technology and society, as well as many ethical considerations of engineering.

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TEM Investigation of Indentation Induced Phase Transformations in Silicon

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Phase transformations induced by nano-indentation have been studied by transmission electron microscopy. Within indentations, a mixture of metastable Si-III (bcc structure) and Si-XII (rhombohedral structure) and their distribution were identified by selected area electron diffraction. The lattice information of metastable silicon phases and the interfaces between crystalline and amorphous materials were investigated by high resolution TEM. A dislocation induced lattice rotation mechanism was proposed to explain the phase transformations and local amorphization in nano-indentation during pressure release.

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Optimization of High Specific Power Electric Machines with Simulated Annealing

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An objective function is a scalar quantification of results with respect to design space variables which evaluates to a lower value at more desirable results. Optimization of relatively complex systems, such as high power electric motors, may require an objective function which contains many local minima within the possible design space. Many optimization routines are only able to find local minima, and will therefore provide different results depending upon the supplied initial point in design space. Global optimization algorithms, such as Simulated Annealing (SA), attempt to escape local minima by allowing "uphill" steps (moves in the design space which result in higher values of the objective function). The process of allowing certain uphill steps is known as the Metropolis algorithm.

In the SA algorithm, steps around the design space are random perturbations from the previous point of evaluation and uphill steps are permitted based on the Boltzmann probability distribution. Just like the annealing, SA relies on a cooling schedule. At higher "temperatures", uphill steps are more readily allowed so that the design space is adequately explored by the optimization routine. As the "temperature" decreases, fewer and fewer uphill steps are allowed until a minimum is found.

This particular SA algorithm utilizes constrained optimization. The random perturbations in the design space can be rejected even before the Metropolis algorithm is considered. Constraints for this design problem include a failure criterion for the composite rotor of the electric machine.

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Gantry Cranes Gain Scheduling Control with Friction Compensation

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Gantry cranes are widely used to transport heavy loads and hazardous materials in factories and nuclear installations. They consist of a trolley, which translates in a horizontal plane. The payload is attached to the trolley by a cable, whose length can be varied by a hoisting mechanism. The load with the cable is treated as a one-dimensional pendulum with one-degree-of-freedom sway.

The objective of crane control is to build an algorithm to move a load from point to point in the shortest time without inducing large swings. We assume that this objective cannot be accomplished in less than a single oscillation cycle of the load. Therefore, the controller is built to move the load such that it completes only one oscillation cycle at the end of the motion. Consequently, the settling time of the system should be equal to the period of oscillation of the load. This criterion enables the calculation of the controller feedback gains for varying load weight and cable length. Numerical simulations show that the controller is effective in reducing the load oscillations and transferring the load in a reasonable time compared with that of optimal control.

In this work, we design our controllers based on a linearized model of gantry cranes. Hence, the nonlinearities, such as Coulomb friction, can not be included. Unfortunately, when the designed controllers are validated on a gantry crane model, it was found that the friction is very high. This friction results in high steady-state error for position control even without swing control. If the swing control is included, the response is completely unacceptable. Therefore, controllers designed based on linear models are not applicable unless the friction is compensated for. This can be done by estimating the friction, then applying an opposite control action to cancel it, which is known as friction compensation. To estimate the friction force, we assume a mathematical model, then we estimate the model coefficients using an off-line identification technique, such as the method of least squares (LS). First, the process of identification is applied to a theoretical model of a DC motor with known friction coefficients. From this example, some guidelines and rules are deduced for the choice of the LS parameters. Then, the friction coefficients of the gantry crane model are estimated and validated.

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The Influence of Broken Fiber Modulus and Slipping Yarn Friction on Stress Concentration in Hybrid Yarns

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Blended or Hybrid yarns, which consist of more than one type of fiber have been produced to develop improved strength and stiffness over what can be achieved in homogeneous yarns. This so called hybrid effect has been observed in hybrid composite sheets, where it is indicated how higher loading and elongation can be sustained by high modulus (low elongation, LE) fibers than when they exist alone in a non-hybrid composite. The same effect is possible for blended yarns. It is shown that the stress concentration factor (SCF) of an LE fiber next to a broken HE (high elongation) fiber decreases, while the SCF of an HE fiber next to a broken LE fiber increases with decreasing values of hybrid parameter, R, the ratio of the axial stiffness of the HE to that of the LE fibers. This has a positive effect for yarns where the principal fibers are particular LE fibers which are selected to be stronger than the dispersed HE fibers. It is suggested that if the reduction of the SCF of the principal LE fiber has a dominant effect on the yarn strength compared with the increase of the SCF of the HE fiber (since the HE fiber usually has a large failure strain), a hybrid effect can be realized.

Near a fiber break, the broken fibers will slip, and the slip extent is seen to play a role similar to the yield zone in the matrix near a fiber break in fiber composites. The friction force on slipping fibers is variable. In the present work it starts from zero at the cut end of the fiber and approaches a constant value with exponential behavior, where the steepness of the approach depends on a parameter, k .The SCF is determined for various values of k . In general,the SCF decreases with smaller values of k and larger slip extents, supporting the notion that slip acts as a dissipative mechanism, similar to matrix yielding in fiber composites.

The present micro-mechanical model is formulated for a blended yarn consisting of LE and HE fibers undergoing axial extension and leads to a system of 2nd order differential equations, which are solved by an eigenvector expansion approach. Solutions are obtained in each of two regions, a region where slip occurs between fibers and one where there is no slip. Appropriate continuity and boundary conditions are then applied in the cases considered.

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Variation of Pressure Gradient Ratio in Dense Phase Pneumatic Transport Systems

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The mode of pneumatic transport very much depends on the nature of the material, but no clear-cut guidelines have yet been established to correlate the mode of transportation with the physical characteristic properties of the bulk solids. Hence, one is compelled to run tests on pilot scale plant with the actual material to be conveyed, and then try to scale up the results for the design of the required plant.

A large number of articles can be found in the literature dealing with calculation technique for pressure drop in pneumatic conveying systems. Many of these techniques depend on conveying trial in a pilot scale test facility. The results obtained are then processed using empirical tools to predict the expected pressure drop of a full scale plant. While calculating the total pressure drop of the system people often differentiate between steady state pressure drop and acceleration pressure drop. Also the steady state pressure drop rate in the vertical conveying and the horizontal conveying is accepted to be different because of additional gravitational force in the vertical pipeline. Naturally, the question arises Is there any relationship between these two pressure drop rates ? If there existed such a reliable relationship then it would be an extremely useful tool for the designers, because then the researchers could undertake experiments using only horizontal test loop and then could predict the pressure drop for the vertical pipes as well. This would eliminate the need for an elaborate test loop. Unfortunately very little published work could be found in the literature in this respect. Although researchers in general agreed that the pressure gradient ratio should be material dependent, they also indicated that the value should be greater than 1.

This paper presents the experimental findings in respect of the pressure drop variation trend in the vertical and horizontal pipe section. The test was conducted with alumina, barite, bentonite and cement as the test materials. Although no clear-cut relationship could be found between the pressure drop gradients, it was possible to find a trend in the variation of the ratio of pressure gradient. The findings of this paper indicate that further work is needed in this direction before a final solution to the problem can be obtained.

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A New Experimental Setup for the Characterization of Bulk Mechanical Properties of Aerated Particulate Systems

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This study introduces the development of a new experimental setup using an enhanced triaxial tester and a new methodology for the characterization of fine particulate systems in an aerated condition. Tests were performed using the new setup to study the effects of aeration on two different powders, i.e. on a highly cohesive precompacted powder and a cohesionless powder. The former being microcrystalline cellulose PH-102, mean particle size 90 micron and the latter alumina powder, mean particle size 100 micron. The degree of aeration was extremely small and it was of the same order of magnitude as the velocities encountered during the entrapment of air in filling and during other handling processes. The superficial velocity for aeration was about 3 orders of magnitude lower than that required for fluidization. The immediate results have shown that even a small amount of interstitial air has a dramatic effect on the quasi-static strength and a considerable effect on the elastic parameters of the powder. In both cases the strength was significantly reduced and there was a noticeable drop in the values of the elastic parameters as well.

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Mesoscopic Structure of Spray Formed High Strength Al-Zn-Mg-Cu Alloys

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High Solute, high strength 7XXX series aluminum alloys with solute contents close to equilibrium solid solubility limits of the Al-Zn-Mg-Cu system have been produced by rapid solidification using spray deposition. This process yields massive preforms directly from the liquid state. Various elements, including chromium, manganese and silver were incorporated to produced a variety of microstructures and mechanical properties. Superior strengths in excess of 860 MPa were achieved and are attributed to two major substructures with different scale; nanometer sized eta prime metastable precipitates and slightly larger, but finely distributed dispersoids. The large volume fraction of plate-like eta prime precipitates were identified as having a hexagonal structure with lattice parameters a = 0.488 and c = 1.376. The remarkable strengthening is predominantly attributed to precipitation hardening and a large coherency strain.

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Multiscale Modeling of Solidification
(Symposium No. 25)

Organizers:
Mark F. Horstemeyer, Sandia National Laboratories
Douglas B. Kothe, Los Alamos National Laboratory

Phase Field Simulations of Dendritic Growth with Fluid Flow

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Understanding the pattern selection process during solidification is an important problem for materials scientists and engineers, as the microstructure formed during solidification affects the properties of the material in service, and cannot be changed readily by subsequent solid-state processing. In this talk, recent computations using phase-field models to directly simulate dendritic growth are described. Where possible, the results are compared with theory and experimental observations.

The important physical phenomena span a range of length scales from a few nanometers to a few millimeters, and this creates a need for advanced computational methods to include the entire range. We employ an adaptive gridding procedure for solving the phase-field equations, where high resolution is available near the interface, and more appropriate grid dimensions are used to resolve the diffusion field.

Recent work examining the role of fluid flow in the pattern selection process will also be presented. Fully three-dimensional simulations of growth of pure materials are presented, and it is demonstrated that the three dimensional aspects of the flow are essential. Parallel implementation of the code is also described. Comparison of computational and experimental results highlights the challenges of both endeavors.

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Investigations of Numerical Methods for Dendritic Solidification

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Fundamental studies of microstructural evolution is a subject of growing impact on fields as diverse as geology, physics, biology, and materials science, to name a few. An important facet in this field is the study of dendritic crystal growth. As such, a variety of different physical models and associated numerical algorithms have been presented in the last decade to study dendritic solidification growth via direct numerical simulation. We present results of a parametric investigation and sensitivity analysis of two-dimensional dendritic crystal growth using two diverse numerical models. We compare our results to microscopic solvability theory. The first, and the most predominant is the phase-field technique. Here a diffuse interface is described by an order parameter ϕ whose evolution is constrained to ensure a monotonic decrease of a free energy functional $\mathcal{F}$. An appropriate choice of $\mathcal{F}$ is required to reproduce the correct jump condition in the limit of a sharp interface. The second method is the front-capturing level set technique which has been used in a variety of moving boundaries applications. In the level set technique, the solid-liquid interface is represented as the zero contour of a distance function. The distance function is used as a computational tool to calculate the correct sharp-interface jump condition to advect the front with. The vehicles we use to investigate these techniques are AMRITA and ADIFOR. AMRITA is a unique combination of a document preparation system, a computational engine (which provides adaptive mesh and parallel capabilities) and a scripting language. This combination allows for extensive parameter studies, comparisons of different numerical algorithms and repeatable investigations to be performed easily. ADIFOR processes numerical codes written in Fortran to provide sensitivities of numerical results to input parameters. These sensitivities can be used directly, as a gradient in an optimization process for fitting data, and/or for quantifying result uncertainties.

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Conduction-Limited Melting of Dendritic Mushy Zones: Experiments & Theory

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Conduction-limited melting processes are of importance in convection-freemelting in low-Earth orbit, during meteoritic genesis, mushy zone fusion, and in welding—all cases where the length scales for thermal buoyancy are restricted. Steady-state crystal growth data reported earlier indicate that dendritic growth under microgravity conditions is limited by diffusional transport. We now report on the melting process, observed for the first time using video images. We observed freezing and melting sequences for ultra-pure pivalic acid (PVA) at different supercoolings. PVA dendrites melt in a stable, afine, manner according to a square-root-of-time dependence. The theoretical kinetics against which the experiment is compared is based on a quasi-static conduction-limited analysis for melting under shape-preserving conditions. The time variable can be nondimensionalized by a Fourier number, $Fo \equiv \alpha t/C_0^2$, where α is the thermal diffusivity of the melt, t is melting time, and C_0 is the characteristic length scale based on the initial length of the dendrite fragment. Comparison between theory and experiment yield Stefan numbers(dimensionless superheating) in agreement with thermal data telemetered from the space-borne thermostat. The experiments and analysis raise questions concerning the rôles of capillarity, kinetics, and convection during melting.

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Simulating Microporosity in an Alloy

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The effect of pressure on the formation of microporosity in an aluminum casting alloy (356) was studied experimentally and by simulations. The finite element simulator is based on a continuum theory of the dendritic solidification of multicomponent alloys. It accounts for the all-solid region, a mushy zone and an all-liquid region of a solidifying alloy. The mushy zone is modeled as a porous medium of varying permeability, where the permeability is a function of the volume fraction liquid and the length scale of the dendritic grains. The complete model comprises component momentum equations, the energy equation, and and one conservation equation for each alloy-element and for the dissolved hydrogen. By solving the redistribution and transport phenomena of hydrogen during solidification and comparing its Sievert's pressure within the solidifying alloy, the simulator predicts whether microporosity forms. The simulator was verified for a set of plate castings of the alloy cast under gas mixtures of argon and 0.2 atm. of hydrogen, with the total pressure set at either 1,10 or 20 atm. The hydrogen was intentionally added to effect microporosity, so that the role of the total on suppressing the microporosity could be studied. It was found that the predicted results agreed reasonably well with experimental measurements of the volume fraction of microporosity. The simulator was also used to show that, with less dissolved hydrogen, total pressures of 10 and 20 atm. can be used to produce castings with no microporosity for the same concentration of hydrogen that yields porous castings that are solidified at 1 atm.

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Modeling of Electron Beam and Laser Welding

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A mathematical simulation software tool is presented to evaluate the effects of fluid flow and temperature field in electron beam and laser welds. The unsteady three dimensional model uses nonuniform hexahedral grids while considering forces such as bouyancy, surface tension and Marangoni effects. Weld pool development and free surface behavior are investigated for various surface tension gradients. Stationary and traveling heat sources are both explored. Simulations are ran for atmospheric conditions and also for vacuum conditions. Results are compared with those found in literature as well as experiments.

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Truchas Models for Flow in Solidifying Systems: Methods and a Validation Example

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Truchas is a computer program under development at Los Alamos National Laboratory for the simulation of various metal processes involving phase change. The program incorporates a variety of physics models, including: electromagnetic heating, flow, heat conduction, liquid-solid and solid-solid phase change, and thermo-mechanical deformation. Its fluid flow models are three-dimensional, unsteady and treat multiple materials, phases and species. Truchas can track interfaces between incompressible fluids as well as between fluids and solids using the Volume of Fluid (VOF) algorithm [1]. The program uses collocated variables in hexahedral non-orthogonal mesh cells. In this paper we describe the flow algorithm used in Truchas, with particular emphasis on those aspects that permit simulation of flow in the presence of liquid-solid phase change. These include the identification of the liquid-solid interface geometry, modification of the volume tracking method to account for this interface, corrections to the viscous stress operator in the vicinity of the interface, evaluation of velocity and pressure gradients near the interface, and use of a porous-medium (Carman-Koseny) drag in the mushy zone formed during the solidification of alloys. Transport of solute concentrations and solidification sources of solute will also be described for metal alloys.

Comparisons will be presented between Truchas simulations and the experimental results of de Groh and Lindstrom [2] for solidification of an ingot of succinonitrile (SCN) in a Bridgman apparatus. SCN is a clear organic material that melts at a convenient temperature and permits observation of the fluid velocity. Experimental data describing the steady state interface shape and the corresponding velocity field will be compared to simulation results in three dimensions.

[1] W.J. Rider and D.B. Kothe, Reconstructing volume tracking, Journal of Computational Physics, 141:112-152, 1998.

[2] H.C. de Groh III and T. Lindstrom, Interface Shape and Convection during Solidification and Melting of Succinonitrile, NASA TM 106487, June 1994.

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Analysis of a Newton-Krylov Scheme for Phase Change Simulation

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The Truchas casting simulation tool under development at Los Alamos National Laboratory incorporates fluid flow, heat transfer, liquid-solid and solid-solid phase change, electromagnetic heating, and thermo-mechanical deformation. Typically, different numerical techniques are required to solve the equations for the various physics models. We describe and present results for the nonlinear solution method used in the heat transfer/phase change portion of simulations, a Jacobian-free Newton-Krylov scheme.

Using the well-known Lazaridis problem[1] we analyze error and present mesh convergence results for a variety of perturbations of the original problem, including both pure and alloy materials, 2D and 3D, and a range of values for the Stefan number.

[1] Lazaridis, A., A Numerical Solution of the Multidimensional Solidification (or Melting) Problem, Int. J. Heat Mass Transfer, 13:1459-1477 (1970).

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Computational Modeling of Polymer Solidification

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We present a theoretical model and computer simulation results describing the solidification process in a polymer due to a curing reaction. The chemical reaction model is based on the model proposed by Kamal and contains power-law terms multiplied by Arrhenius type externally catalyzed and autocatalyzed rate constants. The rate constants and the reaction orders can be derived from experimental techniques like Fourier Transform Infrared spectroscopy (FTIR) or Differential Scanning Calorimetry (DSC). The model was incorporated in the Truchas software tool, developed by LANL's Accelerated Strategic Computing Initiative (code project Telluride). Truchas is a 3D multi-physics, parallel code that was initially designed to simulate manufacturing processes involving flow, phase change, and thermomechanical response of metal alloys. We added a new capability to the code, allowing for the coupling of heat transfer and curing simulations. As an application, we present simulation result of the molding of foam billets consisting of 60 wt% carbon micro-balloons and 40 wt% APO-BMI polymer.

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Verification and Validation of a Casting Simulation Software Tool

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A software tool, called Truchas, is being developed to model the entire metal alloy casting process, from mold preheat and filling to cooling down to room temperature. Key physical models include heat transfer (conduction, convection, radiation) with liquid-solid and solid-solid phase changes, incompressible fluid flow with liquid-gas interface tracking, flow through developing mushy regions, thermal and solutal buoyancy, surface tension effects, thermomechanics, and electromechanics. The specific method for modeling isothermal and non-isothermal phase changes is based on a nonlinear, Newton-Krylov based algorithm of solving an implicit energy equation that uses enthalpy (instead of the more commonly used temperature field) as the dependent variable.

In this talk, we will present some verification and validation results of the Truchas code, with an emphasis on problems involving solidification, through comparison against analytical solutions and experimental data.

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Analysis of Processes Involving Heat Deposition using Constrained Optimization

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We present aspects of a general approach based on constrained optimization for the analysis of processes involving heat deposition such as welding processes. The methodology of this approach entails generating functions and subdomain elliptic solvers useful for the practical application of constrained optimization for the calculation of thermal histories. Our emphasis in this presentation is on the properties of multiscale homogenization, which is the ability to represent fine-scale phenomena via a coarse-scale discretization of physical quantities. Multiscale homogenization is of particular significance for the case of welding processes, which are characterized by temperature fields that have sharp transitions in scale.

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Recent Advances in Ceramic Matrix Composites for Aeronautics & Aerospace

(Symposium No. 26)

Organizer:
Roy M. Sullivan, NASA Glenn Research Center

Overview of Ceramic Matrix Composite Research at NASA for Aeronautics and Space Transportation Applications

Ajay K. Misra*

Chief

This presentation will provide an overview of ceramic matrix composite (CMC) research at NASA for future aerospace applications. Current CMC research activities for gas turbine engine applications include the development of a SiC/SiC combustor liner and turbine vanes that will enable NOX and CO2 emissions. Research efforts for space transportation applications include development of C/SiC and SiC/SiC CMCs for turbomachinery components, actively-cooled structures, and gas generators. The CMC requirements for various applications and progress made toward meeting these requirements will be presented. Key challenges for introduction of CMC's in gas turbine engines and space transportation systems will be discussed.

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Numerical Simulation of Slurry Infiltration of Fiber-Woven Ceramic Composites

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The development of advanced ceramics formed by slurry and melt infiltration of woven preforms is a promising route in producing more energy-efficient engine components, as well as enabling high temperature materials for space propulsion and airframe applications. However, a lack of precise control of processing variables during fabrication gives rise to large variations in mechanical properties, requiring designers to use large knockdowns in design. With a better understanding and control of processing variables one could narrow the property distribution thereby increasing material reliability and durability.

The overall goals of this project are to evaluate the variations at each manufacturing stage, obtain a greater understanding of the infiltration process, and optimize the manufacturing process. This work couples numerical and experimental approaches to develop a model that closely represents the infiltration process and can be used to select optimal architectures and processing parameters. Furthermore, one-dimensional and two-dimensional infiltration models will be compared to determine the accuracy of the assumptions made and results obtained for each.

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Effect of Environment and Material Volume on the Creep-Rupture Behavior of C/SiC

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NASA is developing advanced Reusable Launch Vehicles (RLVs) to replace the Space Shuttle. Within the next 10 years, NASA's goal is to develop a RLV that will reduce the cost of placing payloads in orbit by one order of magnitude, when compared to the performance of the Space Shuttle.

To meet this goal, ceramic matrix composites (CMCs) are proposed for structural propulsion and airframe applications in advanced RLVs due to the higher specific strength and increased temperature margins of CMCs relative to the high temperature materials typically used today, such as superalloys. One candidate CMC material for applications such as nozzles, integrally bladed disks, combustors and heat exchangers is carbon fiber-reinforced silicon carbide matrix composite (C/SiC).

Propulsion components will likely be subjected to service cycles that include mechanical loading under complex environments that include oxygen, hydrogen and steam. To identify the failure modes and degradation mechanisms of C/SiC in these types of environments, stress-rupture tests were conducted in air, vacuum, and steam-containing environments at two temperatures, 600 and 1200C. The failed specimens were examined to correlate the rupture lives with composite damage.

Previous research on the high temperature behavior of C/SiC revealed that oxidation of the carbon fibers is the primary damage mechanism above a temperature of about 400 C. The primary path for oxidation is the matrix cracks present due to the CTE mismatch between the carbon fibers and the SiC matrix. Since the surface-to-volume ratio varies with component geometry, it is important to characterize the effect of cross-sectional area on life. Toward this goal, the stress-rupture behavior of C/SiC was conducted on specimens of three gage section widths. Specimens having gage section widths of 10.1, 17.8, and 25.4 mm were tested to failure at 800 and 1200 C. The creep data for the various specimen widths is compared. Cross-sections of failed specimens were examined to quantify the material damage via fiber oxidation. A low partial pressure of oxygen environment was used for all these tests. The oxygen content of the gases flowing out of the chamber exhaust was monitored as a function of test time. The oxygen content was found to rapidly decrease from the initial value of 1000 ppm during the first 10 % of specimen life and then transition to a steady state value for the duration of the test. The nominal steady state value was inversely related to appled stress.

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Modeling the Oxidation Kinetics of Carbon Fibers Oxidizing in a C/SiC Composite

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Andrew J. Eckel‡ — Materials Research Engineer

A finite difference model was developed to study the oxidation of carbon fibers in a non-reactive cracked silicon carbide matrix. The physics-based oxidation model simulates the diffusion of oxygen into a cracked matrix that is bridged by carbon fiber tows. The cracks are an inherent property of carbon fiber reinforced composites that provide a diffusion path for oxygen to ingress into the composite. The cracks form due to the coefficient of thermal expansion mismatch between the fibers and the matrix.

The model allows the oxygen concentration and carbon volume to be tracked over time. Important variables can be input into the model to simulate different experimental or use conditions. The variables include the oxygen partial pressure, temperature, carbon reaction rate constant, and the diffusion coefficient. The model also allows for different sized matrix crack openings to be input into the model so that the effects of Knudsen diffusion can be considered for small crack openings.

The carbon oxidation patterns and local oxygen concentrations are compared to experimental observations. Two primary oxidation kinetic regimes are identified. In the low temperature range, reaction controlled kinetics are observed. Minimal oxidation is observed throughout the cross-section of the composite even deep in the interior away from the edges. This is due to oxygen diffusing into the material at a faster rate than it can be consumed by reactions with carbon. Oxygen is able to bypass carbon at the perimeter of the cross-section and saturate the interior. In the high temperature range, diffusion controlled kinetics are observed. In this case, a shrinking core effect is seen as oxygen diffuses in from the edges and is quickly consumed by the carbon. A distinct reaction front is observed that moves inward as the carbon is consumed. There is a sharp gradient in oxygen concentration at the reaction front and no oxygen is able to bypass the reaction front. The interior of the composite is starved from oxygen so that it remains unreacted until the reaction front arrives.

The oxidation model is useful in understanding the oxidation of carbon fibers and the oxidation kinetics due to the influence of important variables. Also the model can be used to draw a correlation between carbon consumption and strength reduction and/or time to failure.

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2400F CMC for Gas Turbine Application

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NASA's Ultra Efficient Engine Technology (UEET) program has fabricated a vane subelement demonstration component for gas turbine applications. The vane subelement is fabricated from a silicon melt infiltrated SiC/SiC composite having a peak temperature capability of 2400F. The subelement vane fabrication is the first stage towards completing a full rig test by mid 2005. Fabricated vane sub-elements will be tested in the High Pressure Burner Rig (HPBR) at NASA Glenn in late 2002 to address fabrication and attachment issues. Vane subelements possess a uniform cross-section design, derived from a metal vane design used in an existing gas turbine engine. The preliminary design of a HPBR test section for SiC/SiC vane subelements is complete. Two vendors, GE Power Systems Composites (GEPSC), of Newark, DE, and Goodrich Corp, of Santa Fe Springs, CA, will manufacture the vanes. The fiber preforms for the vanes will be made at NASA with woven cloth and braided structures, obtained from two other vendors. It is anticipated that vanes consolidated by both GEPSC and Goodrich will be tested. The SiC/SiC vanes are to be tested in the HPBR later this year.

In support of planned testing of SiC/SiC vanes, CFD analyses were completed. CFD analyses were performed to determine the boundary conditions for the SiC/SiC vane during testing in the HPBR. The boundary conditions are required to estimate stresses within the part via finite element modeling. The first stage turbine vane subelement will have a simple geometry, i.e. no twist or camber, to simplify analysis, and fabrication. The vane subelement has a chord length of about 2.1 inches. An axial length of 2.5 inches is desirable. Finite element modeling of the vane subelement will be presented and discussed.

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Properties of CMC Composites from the Second Generation RLV Design Methodology Program

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As part of NASA's Second Generation Reusable Launch Vehicle Program, the Ceramic Matrix Composite (CMC) Design Methodology Program is aimed at developing the tools to effectively design robust and reliable CMC structures for a variety of future spacecraft and space propulsion applications. The payoff in high temperature applications and the potential for weight savings make the application of CMCs an enabling technology for many of the advancements in performance now envisioned for the next generation space vehicle. The CMC Design Methodology Program is concentrating on carbon fiber-reinforced silicon carbide (C/SiC). This program is an integrated study involving analysis, material model development, and material testing to provide the basic understanding necessary to design C/SiC components.

This paper will present the results of the material testing phase of the program. Mechanical and thermal properties data for C/SiC composites fabricated with both two-dimensional laminates and three-dimensional weaves will be presented. Refractory Composites Incorporated (RCI) of Glen Burnie, MD and GE Power Systems Composites (GEPSC) of Newark, DE fabricated the material needed for this study. This paper will also discuss the plans for more advanced data generation.

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Nonlinear Analysis of Ceramic Matrix Composites for Aerospace Applications

Brian J. Sullivan*
Director

Carbon fiber-reinforced silicon carbide matrix composites (C/SiC) are being strongly considered for use as the material of choice on several components of re-usable launch vehicles, including the control surfaces of the vehicle and as high temperature turbine engine and exhaust washed structure applications in the propulsion system. Elevated temperature capabilities coupled with low densities are helping to make C/SiC composite structures an attractive alternative to control surfaces employing thermal protection systems and to high temperature refractory metal propulsion system components. However, due to their complex nonlinear stress-strain behavior, designers face significant challenges in using C/SiC materials as the material of choice for highly-stressed applications.

This presentation will discuss relevant nonlinear stress-strain curves of C/SiC composites and review analytical methods for implementing nonlinear material models. The design of a C/SiC structural subelement test, intended to invoke the nonlinear stress-strain response of the material, will be reviewed. Finally, a comparison between mathematical model predictions and the measured response of the C/SiC subelement will be provided. This same test will be used to demonstrate the importance of nonlinear material modeling, through a comparison of calculated responses using linear and nonlinear material models with the actual measured behavior.

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Modeling of a 3-D Angle Interlock C/SiC Composite

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Ceramic matrix composite (CMC) materials are an emerging technology with potential high payoffs in advanced spacecraft and space propulsion applications. The ability of CMCs to maintain strength and stiffness at high temperatures make them attractive in a variety of high temperature applications. The development of CMC technology is considered by many as essential to the realization of a reusable launch system that will meet the requirements of the next generation Space Shuttle. Before CMCs find extensive use in advanced spacecraft and space propulsion applications, their reliability as hot structures capable of withstanding high cyclic stresses in high temperature environments must be established. The development of accurate mathematical models that simulate the thermostructural behavior over a wide temperature range will help to increase the reliability of CMC components, by helping to understand the material's response to loading as well as its fatigue and fracture behavior.

One of the CMC material systems being considered for spacecraft applications is carbon fiber-reinforced silicon carbide (C/SiC). This material is fabricated as both two-dimensional laminates and three-dimensional weaves. Regardless of the type of construction, the matrix in C/SiC composites is always cracked (to some extent) in the as-fabricated state. This is due to the mismatch in the thermal expansion behavior between the fiber and the silicon carbide matrix in combination with the temperature excursions required for processing. Material models for C/SiC must account for the effect of matrix cracking on the thermostructural behavior.

In this study, mathematical models are developed to simulate the thermostructural behavior of advanced three-dimensional woven C/SiC composites. Three modeling approaches are pursued: a micromechanics-based approach using W-CEMCAN (Woven Ceramic Matrix Composite Analyzer), a laminate analogy method (LAMS) and a structural frame approach. All three techniques are applied to predict the thermomechanical properties of a three-dimensional woven angle interlock C/SiC composite. The properties are predicted as a function of temperature and the extent of matrix cracking. General observations regarding the three approaches for composite analysis are discussed and a comparison of the predicted results with the measured data is presented.

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Damping Characteristics of 3-D Reinforced C/SiC Ceramic Matrix Composite

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For future space and aeronautics propulsion systems, the development of ceramic composite integrally-bladed turbine disk (blisk) technology is attractive for a number of reasons. The high strength-to-weight ratio of ceramic composites helps to reduce engine weight and the one-piece construction of a blisk will result in fewer parts count, which should translate into reduced operational costs. One shortcoming with blisk construction, however, is that blisks may be prone to high cycle fatigue due to their structural response to high vibration environments. Use of ceramic composites is expected to provide some internal damping to reduce the vibratory stresses encountered due to unsteady flow loads through the bladed turbine regions. One objective of the Ceramic Matrix Composite (CMC) Blisk Development Program is to characterize the extent to which ceramic composites can damp these vibrations. In particular, a carbon fiber-reinforced silicon carbide (C/SiC) system has been identified as a candidate for this blisk development program.

The goal of the present research is to characterize the dynamic mechanical behavior of 2-D and 3-D braided C/SiC composites. C/SiC samples were produced using a preceramic polymer infiltration and pyrolysis (PIP) process. Dynamic and static mechanical properties were measured. Mechanical property values were found to be comparable to those measured for specimens produced with a chemical vapor infiltration (CVI) process. Damping appeared to decrease with an increase in the natural frequency. Absolute damping at high frequencies was less than 0.2%. While the critical damping amount of approximately 2 % is required for the Space Shuttle Main Engine (SSME) turbopumps, future propulsion systems may require even more. Thus, the present research results suggest that external damping treatments may be required for the advanced high-temperature, high-speed C/SiC turbine blisks.

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Materials Modeling Issues for Engineering Systems

(Symposium No. 27)

Organizers:
David Lo, Sandia National Laboratories
Bill Scherzinger, Sandia National Laboratories

Nucleation and Propagation of an Edge Crack in a Uniformly Cooled Epoxy/Glass Bimaterial

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Technical Staff Technical Staff

An epoxy/glass bimaterial beam test configuration has been used to study cooling-induced crack nucleation and propagation. This effort extends a nucleation criterion, previously applied to tensile-loaded, adhesively bonded butt joints, to another geometry and type of loading. Loading by thermally induced straining complicates the application of a nucleation criterion based upon parameters defining the asymptotic stress fields at the interface edge (i.e. at the edge discontinuity defined by the intersection of the interface and stress-free boundary). In contrast to the tensile-loaded butt joint, where the magnitude of asymptotic stress state is fully characterized by a single interface-edge stress intensity factor K_a, an additional, non-negligible r-independent regular term K_{a0} always exists for thermally induced strains. In the present work, a direct extension of the previously used nucleation criterion is applied: crack nucleation occurs when $K_a = K_{ac}$, but with the stipulation that interface-edge toughness K_{ac} depends on K_{a0}.

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Constitutive Restrictions for a New Class of Models Describing Isotropic, Nonlinearly Hyperelastic Materials

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In classical nonlinear elasticity, the stored-energy of an isotropic hyperelastic material, like rubber, say, can be written as a function of a standard set of invariants for an appropriate strain measure. This approach is mathematically elegant and by it one can solve analytically many basic and interesting boundary-value problems. One the other hand, for determining specific models from experimental data, the use of the standard invariants is problematic. For experiments typically used to collect stress-strain data, like biaxial stretching experiments, a high covariance among the stress response terms propagates experimental error. Consequently, fitting the parameters in the model accurately is difficult.

To address this problem, Criscione et al.[1] developed an alternative set of invariants, based on the logarithmic, or Hencky, strain. Though less elegant mathematically than the standard isotropic invariants, the alternative invariants admit straightforward mechanical interpretations—unlike the standard invariants—and, more importantly, yield models that do not suffer from covariance among the stress response terms. In [1], Criscione et al. demonstrate the use of their alternative invariants to accurately fit models from several classical data sets for biaxial-stretching experiments on rubber.

Although experimental concerns motivated the development of this alternative set of invariants, analyzing the mathematical properties of models based on these invariants is still important. As suggested by [2], such analysis illuminates the mechanical properties of the material described by the model and, by providing additional restrictions on parameters, is helpful for fitting models from data. Which mathematical properties to study are suggested by several constitutive restrictions from nonlinear elasticity. For models based upon the alternative invariants, we consider three classical constitutive restrictions: the Baker-Ericksen inequalities, Hill's inequality, and the strong ellipticity condition. After deriving the precise form that each constitutive restriction takes for the models we consider, we examine the advantages and disadvantages of using the alternative invariants instead of the standard invariants. For some special classes of models based upon the alternative invariants, we derive detailed restrictions on the parameters in the model.

[1] J.C. Criscione, J.D. Humphrey, A.S. Douglas, and W.C. Hunter. An Invariant Basis for Natural Strain which Yields Orthogonal Stress Response Terms in Isotropic Elasticity. *J. Mech. Phys. Solids*, 48:2445–2465, 2000.

[2] J.P. Wilber and J.R. Walton. The Convexity Properties of a Class of Constitutive Models for Biological Soft Tissues, *Math. Mech. Solids*, to appear, 2002.

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A Dilatational Plasticity Theory for Viscoplastic Materials

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The dilatational plasticity theory of Gurson (1977) has been widely used in the study of ductile failure of solids due to void nucleation, growth and coalescence. The Gurson's model, however, is limited to rate-independent materials and cannot be applied to rate-sensitive solids (e.g., material behavior at high temperature). The Gurson's model is generalized in this paper for viscoplastic materials. A unit-cell model of a viscoplastic matrix containing a microvoid is adopted to establish the viscoplastic constitutive relations for voided, dilating materials. Approximate analytic constitutive relations are proposed, which have all the correct asymptotic limits such as the rate-independent plasticity (i.e., Gurson's model), linear visco-elastic solid, pure volumetric deformation, pure deviatoric deformation, vanishing void volume fraction as well as vanishing matrix volume fraction. The numerical results also show that the approximate constitutive relatios agree well with the unit-cell model.

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Challenges in Modeling the Resistance Welding Process

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Resistance welding is used near the final steps in a complicated and expensive manufacturing process related to the fabrication of pressure vessels. In this multi-year project, we are developing validated modeling tools to accurately predict temperature, deformation, residual stress, and microstructural state due to resistance welds. The goal of this project is to optimize the weld process to minimize the residual stress state, and understand how the process and material parameters relate to weld quality.

In the resistance welding process studied here, large forces and high currents are applied to the parts being joined. Arcing across the interface does not occur because the force is applied prior to the electric current. The applied current generates resistance (or Joule) heating and causes the interface to reach near melt temperatures. The material thermally softens and significant plastic deformation (upsetting) occurs. When welded properly, a solid state bond occurs due to diffusion and grain growth across the weld interface.

The electrical, thermal, and mechanical problems are strongly coupled through resistance heating and the ensuing high temperatures and large deformations that occur during the resistance weld process. The material behavior is described by the Bammann-Chiesa-Johnson (BCJ) internal state variable model which accounts for strain rate, temperature, and load path history effects.

Initially, we have applied the process model to the resistance butt-welding of 304 stainless steel tapered bars. Experimental data exists from a previous study in which both large loads and high currents were applied to a single, tapered bar (an interface did not exist). This configuration allows us to concentrate on the fundamental issues of electrical-thermal-mechanical coupling, as well as the large deformation and elevated temperature material response. Predicted temperatures agreed well with experimental temperature histories. The history of axial deformation and the final deformed shape also compared favorably with experiment.

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Structural Dynamics and Stability
(Symposium No. 28)

Organizers:
Eric Mockensturm, The Pennsylvania State University
Arvind Raman, Purdue University

Equilibrium and Belt-Pulley Vibration Coupling in Serpentine Belt Drives

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Serpentine belt drives with spring-loaded tensioners are widely used in the automotive industry to drive vehicle accessories. Experiments show that large span transverse vibration can be excited despite no lateral forces being directly exerted on the spans. This indicates strong linear vibration coupling exists between the pulley rotations (which are directly excited) and the transverse span deflections. Former models that treat the belt as a string and neglect the belt bending stiffness can only explain the coupling between the tensioner and the two adjacent spans but can not explain the above coupling phenomenon because large transverse span response is not limited to these two spans. In this paper, a dynamic serpentine belt system model incorporating belt bending stiffness is established. The model captures a new linear coupling mechanism which can account for the transverse vibration responses for all spans. The finite belt bending stiffness causes non-trivial transverse equilibria for spans, which cause linear span-pulley coupling, and the degree of coupling is determined by the equilibrium curvatures. A numerically exact solution is presented to determine the span and tensioner equilibria. This requires a novel transformation of the governing equations to a standard ODE form readily accepted by general-purpose BVP solver codes. A closed-form singular perturbation solution is also developed for the case of small bending stiffness. A coupling indicator based on the equilibria is defined to quantify the undesirable pulley-belt coupling. Large coupling indicator identifies strong belt-pulley vibration coupling. Effects of the design variables on the coupling indicator are exposed in simple expressions by the perturbation solution. Results show that belt bending stiffness and span tensions strongly influence the pulley-span coupling, speed has a much smaller effect on the coupling for properly designed system, and the effects of tensioner spring stiffness and longitudinal belt stiffness on coupling are negligible. Belt drive geometry plays an important role in coupling. Increasing the radii of pulleys that bound the problem span having large transverse vibration is an effective and low cost solution to troubleshoot coupling-induced vibration problems. The equilibria appear in the dynamic equations of motion for linear vibrations about equilibrium. Belt-pulley coupling in the vibration modes (and the response) depends on the coupling indicator discussed above. The evolution of vibration modes computed using the obtained equilibria confirms the effectiveness of the coupling indicator in measuring the belt-pulley coupling. Coupled dynamic responses of the spans and the pulleys observed in experiments are plausibly explained and predicted by this proposed model.

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Nonresonant Modal Interactions in a Flexible Externally Excited Cantilever Beam

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An experimental and theoretical study of the response of a flexible cantilever beam to an external harmonic excitation near the beam's third natural frequency is presented. We observed that the response includes a large contribution due to the first mode of the beam accompanied by a slow modulation of the amplitude and phase of the third mode. In addition, we noted that the energy transfer between the modes is very much dependent upon the closeness of the modulation (or Hopf) frequency to the first-mode natural frequency. In earlier studies by Nayfeh and coworkers, the modulation frequency was close to the first-mode natural frequency, and therefore large first-mode swaying was observed. But for higher forcing amplitudes, the present experiments show that the modulation frequency tends to shift away from the first-mode frequency, and subsequently very little swaying is observed. We corroborate our experimental findings with a reduced-order analytical model obtained by discretizing the integral partial-differential equation of motion using the Galerkin procedure with a three-mode approximation.

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An Embedded Sensitivity Approach for Diagnosing System-Level Noise and Vibration Problems

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The feasibility of sensitivity analysis for diagnosing system-level noise and vibration problems is examined in this work. Certain components or subsets of components in complex linear systems can be more responsible for introducing noise and vibration problems than others at certain frequencies and a hybrid analytical-experimental 'embedded' perturbation approach can help to identify those component(s) and the most promising potential design modifications for reducing noise and vibration levels. In embedded sensitivity analysis, only an experimentally determined input-output model is assumed to be available; therefore, the functional elements in this model must be combined in unusual ways to extract patterns for diagnosing system-level noise and vibration problems.

Low order lumped parameter linear models of vibrating vehicle systems are first used to explain how these components contribute to specific noise and vibration problems in the neighborhood of system resonant frequencies. Frequency response function analysis and rigid body simulations are both used to demonstrate the contribution of component design parameters to overall system-level input-output characteristics.

A series of examples are used to motivate the use of embedded sensitivity analysis for the purpose of diagnosing system-level vibration problems. Although only one set of measured system input-output functions are available, an appropriate analytical parameterization of these functions leads to simple relationships between the measured functions and the desired embedded sensitivity functions. These relationships are a substantial finding because they suggest that although the inverse problem for source identification is ill-conditioned due to the correlation between the response characteristics of all the components at a mode of the system, there is nonetheless a means for identifying which components are more responsible for a given noise and vibration problem and candidate design modifications for correcting the problem.

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A Theoretical and Experimental Investigation of the Global Dynamics of Buckled Beams

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We investigate the nonlinear vibrations of a clamped-clamped buckled beam. The beam is subjected to an axial force beyond the critical load of the first buckling mode and a transverse harmonic excitation. We solve the nonlinear buckling problem to determine the buckled configurations as a function of the applied axial load. A Galerkin approximation is used to discretize the nonlinear partial-differential equation governing the motion of the beam about one of the buckled configurations to obtain a set of nonlinearly coupled ordinary-differential equations governing the time evolution of the response. These discretized equations are used to investigate the bifurcations of periodic responses of the buckled beam to primary-resonance and subharmonic excitations of the first vibration mode. We found out that using a single-mode approximation leads to quantitative and qualitative errors not only in the dynamic behavior, but also in the static behavior.

For the primary-resonance excitation, we set the excitation frequency to be nearly equal to the natural frequency of the first vibration mode of the buckled beam. Increasing the excitation amplitude leads to a series of supercritical period-doubling bifurcations culminating in chaos of the local attractors. Increasing the excitation amplitude further results in snabthrough and a quasiperiodic motion. We note that quasiperiodic motions cannot be predicted by using a single-mode discretization.

For the subharmonic excitation, we set the excitation frequency to be nearly equal to twice the natural frequency of the first vibration mode. As the excitation amplitude is increased beyond a critical value, we obtain a period-two motion. Increasing the excitation amplitude further results in a Hopf bifurcation, which leads to a new frequency in the response. In general, this new frequency is incommensurate with the excitation frequency, and hence the resulting motion is a two-period quasiperiodic motion. However, if the new frequency is commensurate with the excitation frequency, the resulting motion is a phase-locked motion. In our case, the new frequency is one sixth of the excitation frequency and the resulting response is a period-six motion. The obtained numerical results are in good agreement with the experimental results.

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Nonlinear Modeling and Dynamic Stability of a Uniformly Loaded Thin, Rotating, Circular Disk

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In this paper, we consider the nonlinear modeling and stability of a uniformly loaded, thin, rotating circular disk. The application considered is flexible memory disks such as floppy and Zip disks. In previous literature, the emphasis has been on the nonlinear coupling between the disk and the surrounding fluid (air). In most studies, the modeling of the disk has been linear. Aerodynamic coupling is thought to be crucial to the dynamic stability of these devices, and the past emphasis on this coupling is therefore justified. In this work, however, we consider the behavior of the disk without aerodynamic coupling but loaded uniformly by gravity. We use von Karman's model for nonlinear disk deflection and examine the importance and influence of the free edge boundary conditions in this model. Understanding both the physical implications and numerical difficulties arising from this modeling is essential prior to incorporating the model in more complicated aerodynamically coupled model. Such modeling insights will also be relevant to the modeling of webs and other two dimensional, flexible structures. The resulting stability maps can also help distinguish any advantages to positioning removable data storage disks horizontally or vertically.

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Instability Mechanisms of a Supercritical Flexible Disk Rotating in an Acoustic Cavity

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Rotating flexible disks are principal machine elements in a wide variety of mechanical systems ranging from turbomachinery to information storage devices. Stable, high-precision operation at high speeds can greatly increase the performance and throughput of such systems. However, disk operation at high, supercritical speed is often hampered by the onset of traveling wave aeroelastic flutter instability. In many applications such as in hard disk drives, CD/DVD drives, sawblades, and turbomachinery the rotating disk is enclosed in a cavity and the disk-acoustic cavity interactions are significant.

This paper investigates the acoustic-structure coupling and instability mechanisms of a flexible disk rotating in an acoustic cavity. It is shown that the system features two intrinsically different gyroscopic effects: one describing the gyroscopic coupling between disk and acoustic cavity oscillations and another arising from the disk rotation. A discretization of the weak form of the coupled field equations is facilitated by the use of Green's theorem and through the use of the in vacuo disk modes and rigid wall acoustic modes as basis functions. The discretized dynamical system is cast in the compact form of a classical conservative gyroscopic system. The resulting eigenfunctions are complex and represent coupled structural-acoustic oscillations of the system.

Detailed analysis of the system reveals strong eigenvalue veering phenomena and supercritical speed flutter instabilities. When the forward traveling wave frequency of a disk dominated mode encounters an acoustic dominated mode frequency of the same nodal diameter number, the disk vibration dominated mode veers into an acoustic dominated mode. This in turn coalesces with backward (reflected) traveling wave at super-critical speed thus leading to the onset of traveling wave flutter. Because flutter can occur only in modes that are gyroscopically stabilized following the loss of their positive definiteness, every nodal diameter mode can flutter except the zero and one nodal diameter modes. Interestingly, each mode flutters only over a finite range of rotation speeds and stabilizes again at higher speeds. These describe completely the instability mechanisms of the conservative system.

In the presence of acoustic cavity damping it is shown through the Kelvin-Tait-Chetaev theorem that the disk destabilizes through flutter instability at critical speed, and remains unstable for all super-critical speeds. Finally we conclude that the aeroelastic flutter speed in practical situations of damped disks rotating in damped acoustic cavities is controlled directly through an interplay of cavity and disk damping.

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Combination Parametric Resonance of Nonlinear Circular Plate Subjected to Thermal Loading

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We analyze the nonlinear response of a clamped circular plate with immovable edges to thermal loads, which produce a temperature consisting of a constant component and a harmonically varying component. The plate is modeled using the dynamic analogue of the von Karman nonlinear equations. We determine a second-order approximation of the solution using the method of multiple scales. The solution indicates several interesting features. First, the linear vibration problem of a plate under uniform thermal loading reduces to the problem of classical stability of plates under in-plane loading. This indicates that beyond a critical temperature, the plate buckles. We determined this critical temperature as a function of the plate characteristics. Second, due to the nonlinearity, we found that the plate will undergo large-amplitude responses due to a combination parametric resonance of the additive type involving the first and second modes. The present analysis might be of importance in the design of MEMS devices. These resonances might impact positively or negatively the performance of such devices, depending on the application.

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Vibration of Flex Circuits in Hard Disk Drives

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Professor

A flex circuit connects the stationary electronics components in a hard disk drive to the rotating arm that carries the read/write heads and positions them above data tracks on the disk. Flex circuits are conventionally formed as a laminate of polyimide substrate, adhesive, and copper conductor. The deformations of a flex circuit are discussed in the context of the initial unstressed shape, a configuration in which stresses relax and set in response to elevated temperature, equilibrium, and small amplitude vibration. The model involves displacements of the flex circuit in the directions tangent and normal to the local equilibrum shape, and those motions couple with the arm's dynamics. Non-linearity associated with finite curvature, partial elastic springback, and the arm's geometry and inertia properties are incorporated with the vibration model to predict the system-level natural frequencies, mode shapes, and coupling factors between the circuit and the arm. Laboratory measurements are used to validate the model with respect to the circuit's shape, stiffness, restoring moment, and natural frequencies. In the vibration experiments, a segment of retroreflective tape was attached to the flex circuit so as to improve the displacement and velocity measurements made through non-contact laser interferometry. The primary degrees of freedom for optimizing flex circuit design are the thicknesses of the individual layers within the circuit, free length, and the locations and slopes of the circuit's attachment points to the arm and electronics block. The model's predictions and trends from a case study in free length are discussed with a view toward reducing coupling between the circuit and arm in certain vibration modes.

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Stability of a Supercritical Driveline Connected by Non-Constant Velocity Couplings Subjected to Misalignment and Torque

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With the trend toward high-speed, light-weight supercritical drivelines, it is increasingly important to understand all instability phenomena associated with realistic driveline configurations. Furthermore, it is important to understand the interaction between different instability mechanisms on the overall stability. One well-known instability phenomena that occurs with supercritical shafts is whirl instability due to internal (rotating-frame) shaft damping. Whirl instability occurs at shaft operating speeds beyond the critical speed, and is related to the internal/external damping ratio. Another less explored instability phenomena is parametric instability caused by non-constant velocity (NCV) flexible couplings, e.g. U-Joint or disk-type couplings, common in many drivelines. Some researchers have explored the stability of various single U-joint/shaft-disk systems, where its been shown that misalignment and load-torque generate periodic parametric terms that cause instability near certain shaft speeds. While the results were interesting, the single U-joint system does not really resemble a typical driveline. Furthermore, the effect of the interaction between the different instability mechanisms, i.e. the NCV couplings and the rotating-frame damping on overall driveline stability has not been studied.

The objective of this paper is to investigate the stability of a supercritical driveline connected by NCV couplings subjected to angular misalignment, torsional load-inertia and load-torque. The non-dimensional, periodically time-varying equation-of-motion of a segmented triple-U-Joint driveline with rotating-frame damping is derived. Torsional and lateral shaft flexibly and their effects on shaft speed kinematics are included. Floquet theory is used to explore the effects of internal/external damping ratio, misalignment, load-inertia and load-torque on the stability at sub and supercritical speeds. It is discovered that misalignment and load-torque have both stabilizing and destabilizing effects. Also, it is found that while external damping can stabilize whirl instability, it is not always effective for stabilizing misalignment and torque induced parametric instabilities.

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Large Electroelastic Deformation of an Axisymmetric Dielectric Membrane

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The electromechanical properties of dielectric elastomers, which become polarized once placed in an electric field, have made them an intriguing option for use in artificial blood pumps. Current models of cardiac assist devices mimic the contraction and expansion of the natural pumping chambers of the heart. An electroelastic diaphragm could be designed such that its change in shape in response to an applied voltage will allow it to be the active element of the pump just as the ventricular walls are in the natural heart. It is required that a stroke volume of 70 cc into a systolic blood pressure of 120 mmHg be achieved by the diaphragm. Therefore, it is important to develop a model to characterize the behavior of a thin dielectric membrane to be employed as the active diaphragm within the prosthetic cardiac device. A comprehensive model accounting for large deformations, and the combined elastic and dielectric behavior of an axisymmetric membrane is formulated.

The polarization of the molecular dipoles within the material stores energy in the dielectric medium; this energy can be converted to mechanical energy. A fundamental approach is taken wherefore consideration is given to the internal energy density of the dielectric. Modifications to the elastic model for large deformations of axisymmetric membranes developed by Rivlin and Adkins (1952) are made in order to incorporate the dielectric response resulting from electrostatic forces developed between charged or polarized bodies. As dielectric elastomers are often pre-strained to generate higher forces, the Rivlin and Adkins model is extended to incorporate material pre-strain. The stresses and deformations of the inflated membrane are calculated and the results analyzed. The resulting model shows how system parameters such as undeformed profiles, pre-strain, pressure, electric field, membrane thickness, and edge constraints govern the membrane deformation.

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Dynamic Creep Buckling of Viscoelastic Columns with Large Deformations and Follower Loads - Failure Probabilities and Survival Times

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Professor Emeritus of AAE Intern

Previous investigations of quasi-static creep buckling due to follower loads indicate the significant contributions follower loads play. Equally important effects have been observed in non-follower load linear viscoelastic columns due to inertia loads. In the present paper the effects of inertia are examined for large deformation nonhomogeneous columns with linear viscoelastic responses, large deformations, initial imperfections and quasi-static follower loads. The additional nonlinear contributions due to column end shortening due to both curvature and compressive loads is taken into account. Galerkin's method is used to eliminate spatial variations and the resulting nonlinear temporal governing relations are solved numerically using a fourth order Runge-Kutta approach. Rather than solving the single second order nonlinear differential equation comparable to the elastica, the problem is formulated in terms of three nonlinear coupled first order differential-integral equations describing deflections and angular and shrinking axial coordinates. The linear elastic-viscoelastic integral transform analogy is analytically extended to this nonlinear problem and applies to the formulation of the governing equations, but cannot be easily used in the solution process due to the inherent nonlinearities. The effects of end shortening on elastic and viscoelastic follower load columns are discussed. Column probabilities of failure and survival times due to creep buckling and/or material failure (delamination) are examined in detail including the influence of temperature. Preliminary results show that large deflection linearly viscoelastic columns with quasi-static follower loads under quasi-static conditions exhibit smaller deflections, smaller probabilities of failure and longer survival times than identical columns under the same loads but with dynamic effects caused solely by creep included.

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When Does a Wrinkle Become a Crease?

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The motivation for this study lies in modeling wrinkles and creases that form on rollers during the manufacture of thin film materials such as paper, film, tape, and fabric. Troughs can form in the free spans between rollers due to compressive stresses, which result from tension variations along the rollers. When the troughed material comes into contact with a roller, troughs that do not flatten onto the roller are called wrinkles. As the material is wrapped around the roller, wrinkles can either eventually flatten or become creases.

The web is modeled as an elastica with the independent spatial coordinate aligned with the rotation axis of the roller. Compressive end loads are applied to simulate the compressive stress causing the wrinkle. The model boundaries are the points at which the material contacts the roller. A distributed load acting through the roller rotation axis models the belt-wrap pressure generated by pulling the material over the roller.

Insight into the stability and vibration characteristics of a wrinkle is gained by studying the planar vibration of this model with clamped boundaries. A geometrically nonlinear theory is used to obtain the buckled shape of the beam. This theory is valid for large displacements from the initially flat configuration. The natural frequencies and modes shapes of free, linear vibration about this equilibrium are obtained, using a variational formulation. Ten terms of the unloaded natural vibration modes are used in a Galerkin expansion to obtain convergence of the natural frequencies.

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Steady-Sliding Instability in Fiber Pullout Experiments: Stick-Slip Dynamics of a Two-Sided Contact

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Self-excited oscillations of single-sided contacts have been extensively reviewed in the literature, with special emphasis on steady-sliding instabilities and stick-slip limit cycles. In such systems, a single contact interface with parameter-dependent friction governs the interaction between a slider and a moving surface, with applications in machine tool chatter, position control strategies, and other low-velocity sliding applications. An alternate class of self-excited dynamics problems includes two-sided contacts as seen in plane stress fiber pullout tests and even brake squeal pad/rotor geometries. Systems with two contact interfaces, which can stick and slip independently, possess dynamics substantially more rich than their single-sided counterparts. In this research, a two-sided contact problem is cast in terms of steady-sliding stability, and unstable steady-sliding configurations may lead to complicated dynamics in which the two interfaces do not stick and slip in unison. This is demonstrated through both simple experiments and low-order dynamic models. The results indicate that only certain tuning relationships between the two interface responses are admissible, and these relationships are directly derivable from the interface constitutive behavior.

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Thermomechanics of the Inelastic Behavior of Materials
(Symposium No. 29)

Organizers:
Arun Srinivasa, Texas A&M University
K. R. Rajagopal, Texas A&M University

Thermomechanical Modeling of Dissipative Processes Utilizing a Framework with Multiple Natural Configurations

K. R. Rajagopal*
Professor

Many bodies, both solid and fluid, are capable of being stress-free in numerous configurations that are not related to each other through a rigid body motion. Moreover, it is possible that these bodies could have different material symmetries in these different stress-free "natural" configurations. In order to describe the response of such bodies, it is necessary to know the manner in which these "natural" configuration evolve as well as a class of response functions for the stress that are determined by kinematical quantities that are measured from these evolving natural configurations.A frameworkis developed to describe the mechanics of such bodies whose "natural configurations" evolve during a thermodynamic process. The framework is capable of describing a variety of responses and has been used to describe traditional metal plasticity, twinning, traditional viscoelasticity of both solids and fluids, solid-to-solid phase transitions, polymer crystallization, multi-network polymers, and anisotropic liquids. The classical theories of elastic solids and viscous fluids are included as special cases of the framework.

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An Experimental Study of the Thermo-Mechanical Response of Elastomers Undergoing Scission and Cross-linking at High Temperatures

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When an elastomeric material is held at a fixed uniaxial stretch at a sufficiently high temperature, the applied force relaxes to zero as time increases. If the external force is removed before it is fully relaxed, the material has a permanent stretch. The force relaxation is attributed to time dependent scission of macromolecular network junctions. The permanent stretch is attributed to the time dependent formation of a new network with a new reference configuration formed by macromolecules that detach from the original network, recoil and then re-crosslink. The new network restrains the original network from returning to its original state. These phenomena have important implications when elastomeric components operate at high temperatures, either due to their environment or as a result of energy dissipation due to mechanical work. An appropriate constitutive theory is vital for the engineering analysis of such components. This work presents results from an experimental study that has been carried out as part of the development of a constitutive theory for a commercial grade vulcanized natural rubber.

Results are presented for uniaxial and multi-axial extension for various conditions of deformation control, force control and temperature control. These results are interpreted in the context of various constitutive assumptions.

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On the Modeling of an Anisotropic Fluid within a Multiconfigurational Framework

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This work is based on the notion that certain materials have multiple natural configurations and that their response can be characterized as a class of elastic responses from an evolving set of natural configurations, and used this framework to model the behavior of a class of visoelastic fluids that are isotropic with regard to their viscous as well as their elastic response. Here, we also consider the modeling of anisotropic fluids within the framework.

Anisotropic fluids are invariably modeled within the framework of director theories, and such theories require boundary conditions for the directors for the resolution of boundary value problems. Here we present an approach to the modeling of anisotropic fluids, which is not a director theory; no balance laws for directors are posited nor is there a notion of a director body force, director (or cosserat) stress or director kinetic energy. Thus, the present approach does not require specifying any additional boundary conditions other than that usually specified for viscous fluids, even for flows that involve spatially inhomogeneous fields. Moreover, the framework is based on sound thermodynamical footing, the evolution of the natural configurations being determined by the rate of dissipation of the material. To delineate the efficacy of the theory, we solve a problem associated with a shearing flow of the fluid in which we discuss the tumbling and alignment of certain vectors that represent the axes of anisotropy of the fluid and which may be associated with rod-like structures in the fluid.

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Analysis of the Film Casting Process Using a Continuum Model for Crystallization

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Crystallization plays an important role in a number of commercially important polymer processes, of which film casting is one. Here we simulate the film casting process using a newly developed framework for analyzing crystallization in polymers undergoing deformation coupled with cooling. In film casting the polymer melt is extruded out of a die and is subsequently stretched and cooled, during which crystallization takes place and the polymer transitions from a melt to a semi-crystalline solid. The polymer melt is modeled as a rate type viscoelastic fluid and the crystalline solid polymer is modeled as an anisotropic elastic solid. The mixture region, where in the material is transitioning from a melt to a semicrystalline solid, is modeled as a mixture of a viscoelastic fluid and an elastic solid. The anisotropy of the crystalline phase and consequently that of the final solid depends on the deformation in the melt during crystallization. Specific models are generated by choosing forms for the internal energy, entropy and the rate of dissipation, the second law of thermodynamics along with the assumption of maximization of dissipation is used to determine constitutive forms for the stress tensor and the rate of crystallization. The model developed is applied to the film casting process and the results of the simulation compare well with experimental results.

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A Computational Framework for Consistent Embedding of Scales Arising in Multiscale Modeling of Materials

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Many problems in mechanics of materials involve operation of multiple spatial and temporal scales. The issue of scales becomes more pronounced in the analysis of nanocomposites with embedded nanotubes. Numerical methods that lack the notion of scales become ineffective in modeling such material systems because the widely accepted definition of continuum breaks down at nano scales. This paper presents a novel variational framework that presumes the existence of multiple scales in the problem. Consequently, the numerical scheme emerging from this variational framework inherits this property. We include all important physical phenomenon at the microscale and nanoscale into one computational method. Quite contrary to the conventional computational nesting of information from smaller scales into the larger ones, we use a novel mathematical nesting of scales and develop a computational scheme based on this framework. We highlight how the proposed technique can help bridge the gap between molecular dynamics and continuum mechanics. We present some preliminary numerical results and conclude the talk with ideas on extension of the framework to the modeling of weak discontinuities in nanotubes.

References

[1] Masud, A., A Multiscale Variational Method for Multiscale Modeling of Materials, Proceedings of the First Sino-US Joint Symposium on Multi-Scale Analysis in Material Science and Engineering, June 17-20, Beijing, China, 2002.

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Common Trends in Deformation Of Low Stacking Fault Energy Austenitic Steels

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I. Kireeva* — Professor

Recently, we have studied the mechanical properties and microstructural evolution during deformation of low stacking fault energy austenitic steels, in particular Hadfield manganese steel and AISI 316L stainless steel, in single and polycrystalline forms. The main research thrusts of the experimental studies have been the investigation of orientation, stress state, interstitial (carbon and nitrogen) content, precipitate size dependence of competing deformation mechanisms, microstructural and texture evolution, stages of deformation, and repeated reversed loading. Twinning was observed as a primary deformation mechanism at the onset of deformation in certain orientations. The volume fraction of twinning was increased with increasing carbon concentration but first decreased and then increased by increasing nitrogen concentration. Incoherent precipitates did not suppress twinning but increased the flow stress level. In the orientations that twinning theoretically is impossible, extrinsic stacking faults and very thin twins were observed. In the conditions in which twinning is the case, an upward stress-strain response was evident. Micromechanisms behind the aforementioned observations were explained. The study of both single crystals and polycrystalline materials has provided a better understanding of microstructural evolution in the quest for bridging length scales. In this talk, we will present the common trends in deformation of low stacking fault energy austenitic steels with respect to deformation mechanisms and their interactions, orientation and stress direction dependence.

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Coupled Field Formulations for Mechanics and Diffusion in Crystalline

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This work represents a first step toward the development of a continuum field formulation for the coupled phenomena of diffusion and mechanics in polycrystalline solids. The basis of the formulation lies in lattice-level mechanisms, from which is built a continuum thermodynamic description of processes at micron length scales. Considering self-diffusion, the composition problem is posed in terms of a binary vacancy-atom mixture. For mechanics, isotropic linear elasticity and isothermal conditions are assumed. The coupled constitutive relations for composition and mechanics are formally derived from the underlying thermodynamics. When applied to governing partial differential equations for each subproblem, the fully coupled nature is realized. Under applied tractions or intrinsic stress, the atoms diffuse—in general from surfaces with compressive normal traction to those with relatively tensile normal traction. The flow is also mediated by electric fields via the mechanism of electromigration. In the case of metal interconnect lines in integrated circuit devices, the results of these microscopic processes are manifested in phenomena such as diffusional creep, hillock formation, grain growth, grain boundary motion, void formation and void evolution. These phenomena have a significant impact on the function, performance and failure of metal lines. A computational framework based on the Finite Element Method has been developed to solve the coupled equations. Several numerical examples are presented and comparisons with analytical results are provided where the latter are available.

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A Damage Mechanics Theory Without a Potential Surface

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Assoc. Professor

Damage mechanics theories proposed in the literature use various different damage metrics. But they all have something in common that is the damage potential surface. Several material constants are used to define this potential equation. During the loading and unloading process it determines accumulation of the damage process. In this a paper a new damage mechanics theory is proposed in which there is no need to use a damage potential surface, hence no need for empirical material constants. The new theory uses entropy production as a damage metric. The new theory treats a solid medium as thermodynamic system. As a result it is assumed that, laws of thermodynamics are valid for solids. Damage due to thermo-mechanical, electrical and chemical forces are considered in a unified form.

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Cell and Molecular Bioengineering
(Symposium No. 30)

Organizers:
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Cheng Dong, The Pennsylvania State University

Mechanosensing Via Membrane-lipid Perturbations

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Endothelial cells (ECs) form the inner lining of the blood vasculature and are exposed to shear stress (τ), the tangential component of hemodynamic forces. ECs transduce Tau into biochemical processes possibly via EC-membrane perturbations. We have used confocal-FRAP on the DiI-stained plasma membranes of confluent cultured bovine aortic ECs (BAECs) to investigate the effects of Tau on EC-membrane lipid dynamics. We showed: (i) τ induces a rapid, spatially heterogeneous, and time-dependent increase in the lateral diffusion of the fluorescent lipoid probe in the BAEC membrane, and (ii) the location, magnitude, and persistence of these τ-induced increases in membrane fluidity depend on the τ-magnitude and the rate of change of τ. We now present evidence for membrane-phase specificity of lipoid dyes (DiIs) in confluent endothelial cells using confocal molecular spectroscopy. Our measurements of fluorescence lifetime (FL) and polarization (FP) of DiI's in BAEC cell membranes are consistent with the partitioning of DiI C12 (a carbocyanine dye with dual 12-carbon alkyl chains) in a liquid phase of the plasma membrane (FL $\sim$ 0.6 ns, FP $\sim$ 0.06), and of DiI C18 (a carbocyanine dye with dual 18-carbon alkyl chains) in the liquid-ordered or gel phase (FL $\sim$ 1.0 ns, FP $\sim$ 0.3). Fluorescence spectroscopic measurements of membrane-phase specific lipoid dyes allow the quantitative measurements of τ-induced changes in lipid dynamics which have been correlated to changes in biochemical processes in ECs.

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Bone Cell Mechanobiology

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Bone adapts to the mechanical loads to which it is exposed. However, the mechanisms by which this occurs are only partly understood. Our laboratory has been focusing on fluid flow as a potential transducer of mechanical load to bone cells. The majority of studies published to date on the effects of fluid flow on bone cells have applied either steady flow or pulsatile flow. However, physiologic fluid flow resulting from the repetitive loading of daily activities is oscillatory in nature. We have demonstrated that oscillating fluid flow (20dynes/cm2) increases cytosolic Ca2+ concentration ([Ca2+]), p38 and ERK1/2 MAP kinase activity in osteoblastic cells. To examine the relevance of this signal transduction, we examined the effect of oscillating fluid flow on osteopontin mRNA levels in the presence and absence of inhibitors of Ca2+ mobilization and MAP kinase activity. Thapsigargin, which empties cytosolic stores of Ca2+, completely blocked the effect of fluid flow on osteopontin mRNA. A similar effect was achieved with the p38 inhibitor SB203580 and ERK inhibitor PD90859. Interestingly, the putative stretch activated channel blocker gadolinium chloride did not affect the osteopontin response. Thus, both cytosolic Ca2+ and MAP kinase are part of the signal transduction mechanism by which fluid flow regulates osteopontin mRNA. Our laboratory is also interested in the role of gap junctions in sensitizing cellular networks to mechanical signals. Gap junctions are membrane spanning channels that facilitate intercellular communication by allowing small signaling molecules to pass from cell to cell. We have previously demonstrated that gap junctional intercellular communication (GJIC) contributes to bone cell sensitivity to hormonal (parathyroid hormone) and biophysical (electromagnetic fields) signals. Recently we examined the role of GJIC in bone cell responsiveness to fluid flow. Osteoblastic cells expressing reduced GJIC, as a result of expressing antisense cDNA for Cx43, the predominant gap junction in bone, or a dominant/negative Cx43, display a reduced prostaglandin response to oscillating fluid flow. Interestingly, fluid flow-dependent increases in [Ca2+] were not dependent on GJIC. Taken together these results suggest that both cytosolic Ca2+ mobilization and GJIC play important roles in bone cell responsiveness to physiologically relevant mechanical signals. Thus, both may be important targets for developing strategies to increase bone cell sensitivity to mechanical signals.

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Strategies for Microneedle Enhanced Drug Delivery and Biomedical Sensing

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Utilizing current Micro Electro Mechanical Systems (MEMS) technologies, different microneedle designs have been fabricated and integrated with various microfabricated microfluidic devices. Microneedle technology promises to revolutionize health care by allowing the precise injection of therapeutic agents to prescribed locations below the skin. In addition, microneedles can be used for sample collection for biological analysis, delivery of cell or cellular extract based vaccines, and sample handling providing interconnection between the microscopic and macroscopic world. Microneedles are desired because the small size and extremely sharp submicron tip radii reduce both insertion pain and tissue damage in the patient. Microneedles may be used for low flow rate continuous drug delivery such as the continuous delivery of insulin to a diabetic patient. Microneedles may be a variety of sizes and shapes since the needles are defined lithographically as opposed to being machined as a single part. Three different aspects of the microneedle field are examined. The first expands upon prior work on micromolded polysilicon microneedles with improved microneedle fabrication. Fluid flow in microneedles is studied, analyzed, and compared from experimental, theoretical, and computational viewpoints. The second area is the development of a microdialysis needle capable of separating small organic molecules from complex biological solutions. The microdialysis needles were designed and fabricated together with analytical modeling to describe diffusion across semi-permeable membranes. Experiments verify the permeability of the diffusion membranes. Finally, an integrated planar microfluidic system capable of sampling and analyzing biological solutions with feedback controlled drug delivery in response to metabolite levels is examined. The integrated microfluidic system includes the assembly of microneedles with on-chip flow channels and electronics together with previously designed positive displacement micropumps, microvalves and a planar electrochemical sensor for biological detection. Multichannel fluidic control for biological sampling, sensor cleansing and recalibration is demonstrated with integrated sensor operation. Microneedles are integrated for both biological sampling through the microdialysis needle as well as continuous and controllable drug delivery profiles. The microneedles were integrated into a short-term drug delivery device capable of delivering therapeutics intradermally.

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Side-view Imaging and Analysis of Cell Adhesion to ICAM-1 in Shear Flow

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Cell deformation and adhesion in shear flow are important in understanding the mechanism of cellular interaction with a vessel wall. Conventional parallel-plate flow chambers are often used to study cell interactions with different surfaces. However, some important cell deformation and adhesion measurements related to cell-surface contact under flow conditions are difficult to obtain quantitatively. In this study, we have developed an in vitro side-view imaging technique to study the mechanics of T-leukemic cell deformation and adhesion to an ICAM-1 bound surface in shear flow. Human T-leukemic Jurkat cells were selected as an experimental model for the study. Jurkat cells express high levels of beta2-integrins similar to those expressed on the human leukocytes, which are a ligand for ICAM-1, one of the important endothelial adhesion molecules. A novel design of the side-view flow chamber consisted of two precision rectangular glass tubes called microslides. A smaller slide was inserted into a larger one to create a flow channel with a flat surface on which ICAM-1 molecules were present. Two optical prisms with a 45-degree chromium-coated surface were used along the flow channel to generate side-light illumination. The site densities of ICAM-1 absorbed onto the glass surface was quantified by 125I-radioimmunoassay. Flow was generated by a perfusion pump. A 3-D flow field with shear stresses acting on the adherent cells within the flow channel was calculated by using the FIDAP finite element software. Side-view images of Jurkat cells that attached to ICAM-1 (250-700 sites/um2) at shear stresses ranging from 0.5-15.0 dyn/cm2 were studied. Images have revealed that the cell-substrate contact length steadily increased with time during the initial cell attachment to the surface, and subsequently decreased with time as the trailing edge of the cell membrane detached from the substrate, followed by an initiation of cell peeling away from the surface. Changes in cell deformability and adhesive strength to the substrate resulted in significant changes in cell peeling time and contact length under flow conditions. The maximum shear stress acting on a 3-D cell body was found to be 2-4 times of the upstream wall shear stress, influenced by the extent of cell deformation within the flow channel. The horizontal fluid-drag force on a deformed cell was found nearly an order of magnitude smaller than the force acting on a rigid sphere that had the same volume of the cell. Hence, cellular deformation aids to the adhesion process by helping to balance the adhesive and hydrodynamic forces, which affects the transients in cell-surface contact and adhesion strength. The novel applications of the side-view imaging technique provide a useful means to study how cell deformability affects cell adhesion mechanics.

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Submolecular Changes in Fibrinogen Conformation on Model Biomaterial Surfaces

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The interactions between plasma proteins and synthetic materials are a key determinant of the biological response to implanted biomaterials. Fibrinogen is a critical protein in surface-induced thrombus formation due to its role in mediating platelet adhesion to biomaterials by serving as an adhesive ligand for the GPIIbIIIa integrin receptor on platelets. This function is performed by a pair of dodecapeptide ligands located at both ends of the molecule in regions termed the D domains. The adsorption and function of fibrinogen have been widely studied by a variety of techniques, and these studies have demonstrated both time- and material-dependent functional and structural properties of the protein. In this study, we utilize atomic force microscopy (AFM) to examine changes in the individual domains that make up the protein following adsorption to two model biomaterial surfaces.

Fibrinogen was adsorbed from dilute solutions (500 ng to 2 ug/ml) in 1mM phosphate buffer. The two model substrates used in this study were highly ordered pyrolytic graphite (HOPG) a hydrophobic, ultrasmooth material and muscovite mica, a hydrophilic, negatively charged ultrasmooth material. All AFM imaging was done under buffer using a fluid cell on a Multimode AFM (Digital Instruments).

Results demonstrate that fibrinogen denatured much more rapidly and to a greater degree on a hydrophobic graphite surface than on a hydrophilic mica surface, as might be expected from the increased nonspecific interactions the protein will experience. The characteristic D-E-D trinodular structure was readily visible within the protein molecule. Analysis of these individual domains demonstrated differences in the rate of structural change (spreading) within the molecule itself, with increased spreading in the D domain. These results are consistent with the D domain possessing a greater number of hydrophobic residues than the E domain, with increased non-specific spreading as a result of hydrophobic interactions. Spreading of the D domain on graphite was seen out to 2 hours, while the D domain on HOPG and the E domain on both substrates showed no additional spreading after 30 minutes.

These results demonstrate spreading of adsorbed fibrinogen molecules on hydrophobic surfaces compared to polar hydrophilic materials, particularly in the relatively hydrophobic D domains. The role that spreading plays in exposure of functional epitopes in the D domain remains to be seen, but these studies represent an important step towards measurement of structure/function relationships in surface-adsorbed proteins.

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Harnessing Kinesin Motor Proteins for Force Generation and Nanoscale Transport Along Immobilized Microtubule Tracks

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Kinesins are biological motors that transport cargo unidirectionally along intracellular tracks called microtubules. These enzymes, which consist of two motor domains with dimensions 4 nm by 4 nm by 7 nm that are connected to a cargo attachment domain, are attractive candidates for carrying out biomolecular separations, directed assembly of nanoparticles, or for powering microscale devices. Fueled by the chemical energy derived from ATP hydrolysis, conventional kinesin moves at nearly 1 micron/s and individual motors can produce 7 pN of force. However, a prerequisite for harnessing kinesins is properly aligning the microtubule tracks that they walk along. Using protein engineering and biochemical separations, kinesin motors and tubulin protein can be purified, reconstituted in vitro, and observed under fluorescence microscopy. We are developing an approach for immobilizing long (50-100 micron) microtubules on surfaces. In conjunction with these aligned tracks, kinesin motors will be attached to nanoscale particles or microfabricated structures and brought in contact with their conjugate tracks. Towards this goal, we have developed a method for constructing an array of parallel, aligned microtubules on a two-dimensional surface by immobilizing short microtubule seeds, polymerizing long microtubules uniquely from one end, and then attaching the elongated filaments to the surface. One key challenge that we have solved is passivating regions of the surface so that the microtubule seeds adsorb only to desired locations. A second challenge to creating this microtubule array has been to align the elongated microtubules through fluid flow and surface adsorption. By producing a field of aligned microtubules, this array provides a launching point for employing kinesins for directed assembly or nanoscale force generation.

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